



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:09 PM UTC

PDB ID : 8P9Y / pdb_00008p9y
EMDB ID : EMD-17578
Title : SARS-CoV-2 S protein S:D614G mutant in 3-down with binding site of an entry inhibitor
Authors : Adhav, A.; Forcada-Nadal, A.; Marco-Marin, C.; Lopez-Redondo, M.L.; Llacer, J.L.
Deposited on : 2023-06-06
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

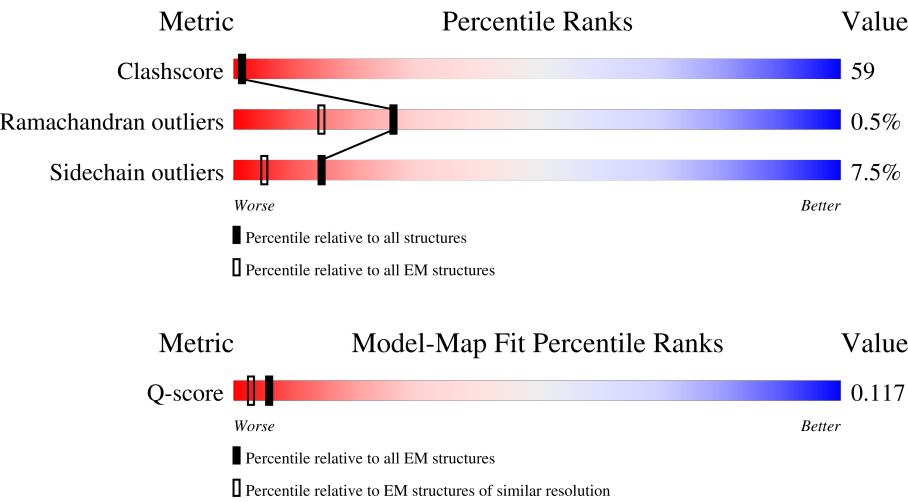
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



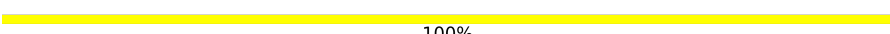
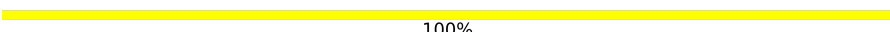
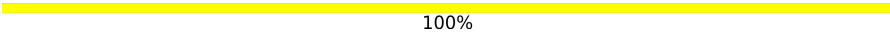
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1270	9% 42% 38% 5% 15%
1	B	1270	41% 39% 5% 15%
1	C	1270	5% 40% 38% 6% 15%
2	D	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	 50%50%
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 50%50%
2	I	2	 100%
2	J	2	 50%100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	I	1	X	-	-	-
2	NAG	L	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1,Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1080	Total	C	N	O	S	0	0
			8425	5378	1403	1606	38		
1	B	1081	Total	C	N	O	S	0	0
			8426	5379	1403	1606	38		
1	C	1076	Total	C	N	O	S	0	0
			8374	5346	1395	1595	38		

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	SER	-	expression tag	UNP P0DTC2
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	ILE	-	expression tag	UNP P0DTC2
A	0	VAL	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	TYR	-	expression tag	UNP P0DTC2
A	3	VAL	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	ALA	-	expression tag	UNP P0DTC2
A	7	ALA	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	HIS	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	PHE	-	expression tag	UNP P0DTC2
A	14	ALA	-	expression tag	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	ILE	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLU	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLN	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	TYR	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	LYS	-	expression tag	UNP P0DTC2
A	1236	ASP	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	TRP	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	PHE	-	expression tag	UNP P0DTC2
A	1242	LEU	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	THR	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	GLN	-	expression tag	UNP P0DTC2
A	1260	LYS	-	expression tag	UNP P0DTC2
A	1261	LEU	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	GLU	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	LEU	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2
B	-3	SER	-	expression tag	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	ILE	-	expression tag	UNP P0DTC2
B	0	VAL	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	TYR	-	expression tag	UNP P0DTC2
B	3	VAL	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	ALA	-	expression tag	UNP P0DTC2
B	7	ALA	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	HIS	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	13	PHE	-	expression tag	UNP P0DTC2
B	14	ALA	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	VAL	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	SER	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	ILE	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLU	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLN	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	TYR	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	LYS	-	expression tag	UNP P0DTC2
B	1236	ASP	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	TRP	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	PHE	-	expression tag	UNP P0DTC2
B	1242	LEU	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	THR	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	LEU	-	expression tag	UNP P0DTC2
B	1247	SER	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	GLN	-	expression tag	UNP P0DTC2
B	1260	LYS	-	expression tag	UNP P0DTC2
B	1261	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	GLU	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	LEU	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	VAL	-	expression tag	UNP P0DTC2
C	-3	SER	-	expression tag	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	ILE	-	expression tag	UNP P0DTC2
C	0	VAL	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	TYR	-	expression tag	UNP P0DTC2
C	3	VAL	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	ALA	-	expression tag	UNP P0DTC2
C	7	ALA	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	HIS	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	13	PHE	-	expression tag	UNP P0DTC2
C	14	ALA	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	VAL	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	SER	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	ILE	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLU	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLN	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	TYR	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	LYS	-	expression tag	UNP P0DTC2
C	1236	ASP	-	expression tag	UNP P0DTC2
C	1237	GLY	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	TRP	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	PHE	-	expression tag	UNP P0DTC2
C	1242	LEU	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	THR	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	LEU	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	GLN	-	expression tag	UNP P0DTC2
C	1260	LYS	-	expression tag	UNP P0DTC2
C	1261	LEU	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	GLU	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	LEU	-	expression tag	UNP P0DTC2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

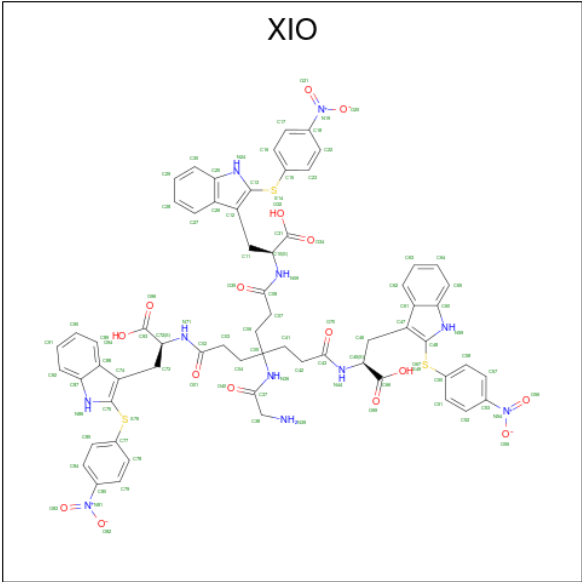
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

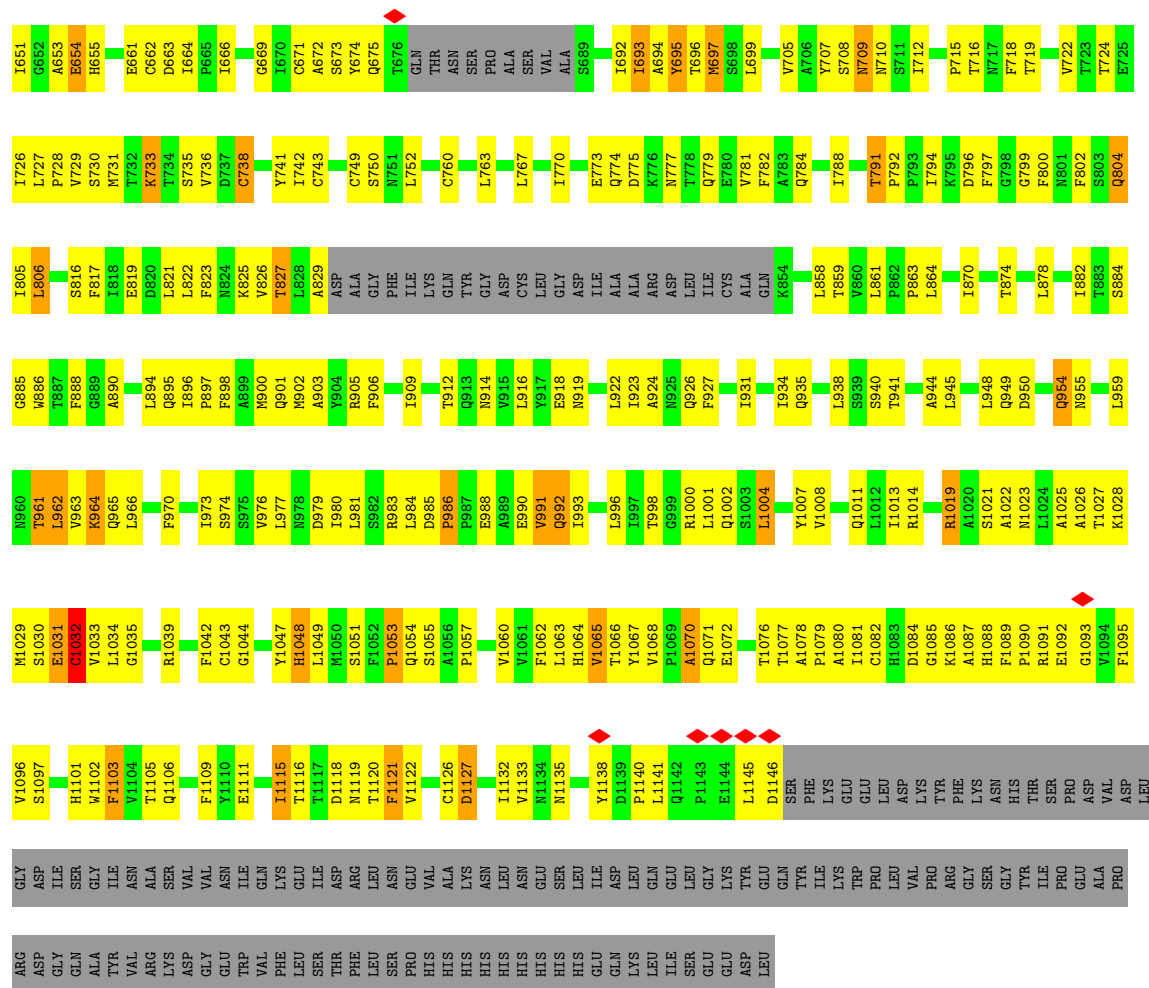
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Na	0
			2	2	
4	C	1	Total	Na	0
			1	1	

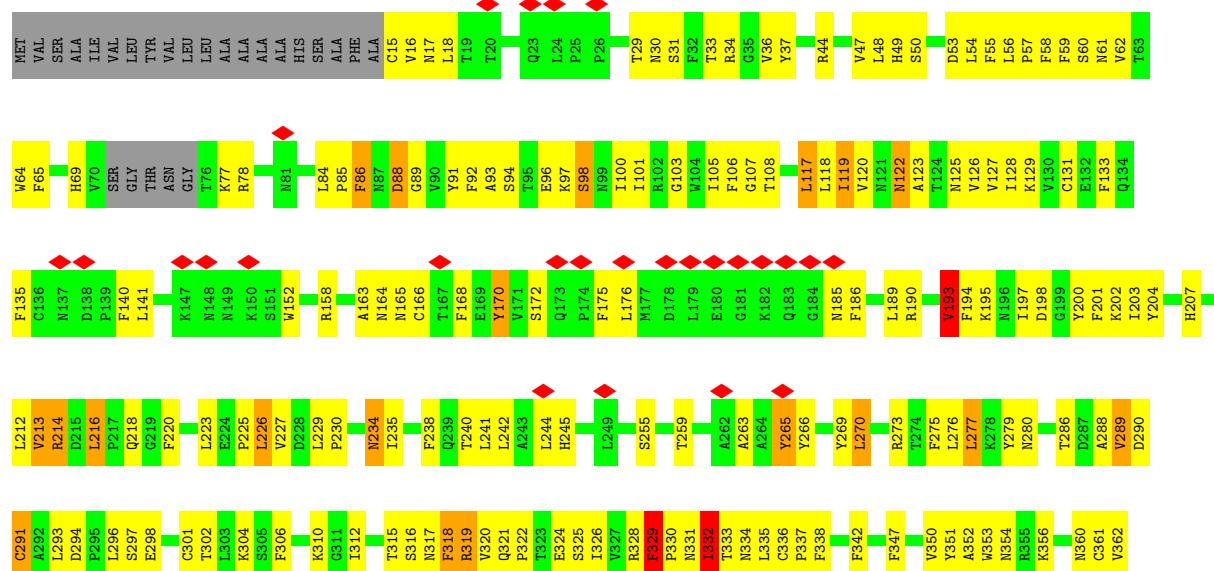
- Molecule 5 is [(2 {S})-2-[[4-(2-azanylethanoylamino)-7-[[[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-4-[3-[[[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-3-oxidanylidene-propyl]-7-oxidanylidene-heptanoyl]amino]-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]propanoyl]oxysodium (CCD ID: XIO) (formula: C₆₃H₅₉N₁₁O₁₆S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	C	1	93	63	11	16	3	0



• Molecule 1: Spike protein S1, Spike glycoprotein





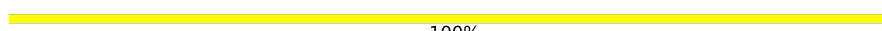
NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50%
100%

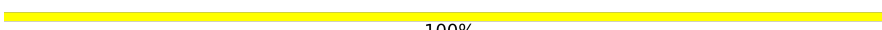
NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

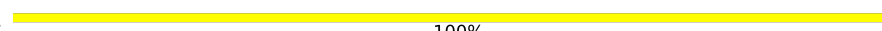
NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97094	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.867	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	420.66, 420.66, 420.66	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NA, XIO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.72	9/8624 (0.1%)	0.97	30/11744 (0.3%)
1	B	0.78	10/8625 (0.1%)	1.00	33/11746 (0.3%)
1	C	0.70	6/8570 (0.1%)	1.01	28/11670 (0.2%)
All	All	0.73	25/25819 (0.1%)	0.99	91/35160 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	940	SER	C-O	-29.95	0.88	1.24
1	A	940	SER	C-O	-22.37	0.94	1.24
1	B	617	CYS	C-O	-11.75	1.09	1.24
1	A	617	CYS	C-O	11.20	1.38	1.24
1	C	676	THR	C-O	-11.18	1.01	1.23
1	C	330	PRO	CA-C	10.11	1.64	1.52
1	A	529	LYS	CA-C	-8.20	1.43	1.53
1	A	1146	ASP	C-O	7.91	1.39	1.23
1	B	676	THR	C-O	-7.17	1.09	1.23
1	B	515	PHE	C-O	-7.15	1.15	1.24
1	B	319	ARG	C-O	-6.65	1.15	1.24
1	A	343	ASN	CA-C	6.56	1.60	1.53
1	C	330	PRO	C-N	6.45	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLY	N-CA	-6.31	1.36	1.45
1	C	488	CYS	CA-CB	-5.96	1.42	1.53
1	B	320	VAL	CA-C	-5.80	1.45	1.52
1	A	530	SER	N-CA	-5.55	1.38	1.46
1	B	516	GLU	N-CA	5.52	1.53	1.45
1	C	331	ASN	N-CA	5.40	1.55	1.46
1	A	98	SER	N-CA	-5.23	1.40	1.46
1	B	98	SER	N-CA	-5.20	1.40	1.46
1	B	320	VAL	C-O	-5.19	1.18	1.24
1	B	592	PHE	N-CA	-5.18	1.37	1.46
1	A	118	LEU	N-CA	5.12	1.52	1.46
1	C	169	GLU	CA-C	-5.00	1.46	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	GLY	CA-C-N	20.38	140.35	119.56
1	C	526	GLY	C-N-CA	20.38	140.35	119.56
1	B	515	PHE	O-C-N	-13.35	104.84	122.59
1	A	1146	ASP	CA-C-O	-11.43	101.37	120.80
1	B	617	CYS	CA-C-O	-10.98	107.69	120.10
1	A	617	CYS	CA-C-O	-10.80	107.90	120.10
1	B	490	PHE	CA-C-N	10.69	130.51	118.85
1	B	490	PHE	C-N-CA	10.69	130.51	118.85
1	C	989	ALA	N-CA-C	-9.09	101.29	112.38
1	A	529	LYS	CA-C-N	-8.82	107.80	121.56
1	A	529	LYS	C-N-CA	-8.82	107.80	121.56
1	A	617	CYS	O-C-N	8.76	132.47	122.22
1	B	617	CYS	O-C-N	8.46	132.12	122.22
1	B	1139	ASP	CA-C-N	8.44	130.39	119.84
1	B	1139	ASP	C-N-CA	8.44	130.39	119.84
1	B	320	VAL	N-CA-C	-8.40	96.02	108.12
1	B	319	ARG	CA-C-N	-8.36	111.36	122.99
1	B	319	ARG	C-N-CA	-8.36	111.36	122.99
1	B	1138	TYR	N-CA-C	8.24	120.27	111.28
1	B	961	THR	N-CA-C	-7.87	102.65	111.07
1	C	208	THR	CA-C-N	7.80	127.35	118.85
1	C	208	THR	C-N-CA	7.80	127.35	118.85
1	B	193	VAL	CB-CA-C	7.68	119.87	110.73
1	B	319	ARG	O-C-N	-7.58	112.70	122.78
1	A	1065	VAL	N-CA-CB	7.47	119.52	111.00
1	B	329	PHE	N-CA-C	7.38	120.06	108.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LEU	N-CA-C	7.29	120.37	108.55
1	C	330	PRO	O-C-N	-6.97	114.21	122.86
1	A	293	LEU	N-CA-C	6.82	118.72	111.28
1	A	308	VAL	N-CA-C	6.63	117.45	108.17
1	A	1032	CYS	CA-CB-SG	6.54	129.45	114.40
1	C	826	VAL	N-CA-C	6.38	113.04	106.21
1	A	986	PRO	N-CA-C	6.37	118.47	110.70
1	A	119	ILE	N-CA-C	6.27	119.09	108.86
1	A	161	SER	N-CA-C	6.22	117.86	111.14
1	A	163	ALA	CA-C-N	6.21	129.74	120.31
1	A	163	ALA	C-N-CA	6.21	129.74	120.31
1	B	1132	ILE	N-CA-C	6.20	118.04	108.44
1	B	590	CYS	CA-CB-SG	-6.19	100.15	114.40
1	A	530	SER	N-CA-C	-6.09	101.53	110.42
1	C	825	LYS	CA-C-N	-6.02	115.99	121.65
1	C	825	LYS	C-N-CA	-6.02	115.99	121.65
1	B	818	ILE	N-CA-C	-5.93	104.73	110.42
1	C	959	LEU	N-CA-C	-5.86	104.97	111.36
1	A	791	THR	CA-C-N	5.70	126.25	120.38
1	A	791	THR	C-N-CA	5.70	126.25	120.38
1	B	1070	ALA	N-CA-C	5.70	117.29	111.14
1	C	856	ASN	N-CA-C	5.67	117.97	107.60
1	A	617	CYS	N-CA-C	5.66	118.22	111.71
1	C	1124	GLY	N-CA-C	5.65	117.61	110.38
1	B	466	ARG	CA-CB-CG	5.62	125.33	114.10
1	A	1031	GLU	N-CA-C	5.58	117.16	111.14
1	B	491	PRO	N-CA-C	5.51	120.78	113.40
1	A	480	CYS	N-CA-C	5.50	116.95	111.07
1	B	291	CYS	N-CA-C	5.49	117.26	111.28
1	A	212	LEU	N-CA-C	5.47	118.98	111.54
1	B	213	VAL	N-CA-C	5.46	116.24	110.72
1	A	806	LEU	CA-C-N	5.46	125.45	119.89
1	A	806	LEU	C-N-CA	5.46	125.45	119.89
1	C	331	ASN	N-CA-C	5.41	116.79	109.11
1	A	733	LYS	N-CA-C	-5.41	101.90	109.96
1	B	468	ILE	N-CA-C	5.32	117.52	111.88
1	B	329	PHE	CA-C-N	5.29	126.46	119.84
1	B	329	PHE	C-N-CA	5.29	126.46	119.84
1	B	170	TYR	N-CA-C	5.28	116.43	108.46
1	C	587	ILE	CB-CG1-CD1	5.25	124.82	113.80
1	C	119	ILE	N-CA-C	5.24	117.60	108.90
1	A	1070	ALA	N-CA-C	5.22	117.05	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	THR	N-CA-C	5.22	117.95	109.24
1	B	84	LEU	CA-C-N	5.21	125.62	119.99
1	B	84	LEU	C-N-CA	5.21	125.62	119.99
1	A	529	LYS	CA-C-O	5.21	127.76	120.52
1	B	642	VAL	N-CA-CB	5.20	118.24	110.13
1	B	466	ARG	N-CA-C	5.19	117.27	109.23
1	C	84	LEU	CA-C-N	5.19	125.09	119.85
1	C	84	LEU	C-N-CA	5.19	125.09	119.85
1	C	1089	PHE	CA-C-N	5.17	124.93	119.76
1	C	1089	PHE	C-N-CA	5.17	124.93	119.76
1	C	103	GLY	N-CA-C	5.16	118.65	110.96
1	A	205	SER	N-CA-C	5.15	117.21	109.23
1	C	520	ALA	CA-C-N	-5.12	114.48	119.76
1	C	520	ALA	C-N-CA	-5.12	114.48	119.76
1	A	130	VAL	CB-CA-C	-5.11	104.08	111.19
1	C	1049	LEU	N-CA-C	5.09	117.96	111.69
1	C	1141	LEU	N-CA-C	5.09	116.83	111.28
1	C	1119	ASN	N-CA-C	5.08	116.90	111.36
1	C	734	THR	CA-C-N	-5.07	115.95	123.05
1	C	734	THR	C-N-CA	-5.07	115.95	123.05
1	C	1108	ASN	N-CA-C	5.05	116.87	111.36
1	A	595	VAL	N-CA-CB	5.03	118.09	111.25
1	B	214	ARG	N-CA-C	5.02	117.49	109.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Mainchain
1	B	515	PHE	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8425	0	8181	955	0
1	B	8426	0	8179	1096	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8374	0	8124	1042	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	A	126	0	117	2	0
3	B	126	0	117	2	0
3	C	84	0	78	1	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	C	93	0	0	0	0
All	All	25937	0	25046	3010	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (3010) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HA	1:C:58:PHE:CE1	1.28	1.65
1:C:541:PHE:CZ	1:C:587:ILE:HD13	1.31	1.61
1:B:543:PHE:CB	1:B:576:VAL:HG21	1.17	1.60
1:A:317:ASN:HB3	1:A:592:PHE:CZ	1.36	1.56
1:B:543:PHE:HB3	1:B:576:VAL:CG2	1.31	1.55
1:B:426:PRO:HG2	1:B:464:PHE:CZ	1.50	1.47
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	1.50	1.43
1:C:516:GLU:HG3	1:C:519:HIS:NE2	1.28	1.43
1:C:33:THR:CA	1:C:58:PHE:HE1	1.34	1.41
1:B:353:TRP:CZ3	1:B:466:ARG:HB2	1.55	1.40
1:B:353:TRP:CH2	1:B:466:ARG:HB3	1.57	1.36
1:C:598:ILE:HD11	1:C:666:ILE:CD1	1.56	1.35
1:B:426:PRO:HG2	1:B:464:PHE:CE1	1.61	1.35
1:A:621:PRO:CB	1:A:637:SER:OG	1.72	1.35
1:B:985:ASP:O	1:B:989:ALA:HB2	1.24	1.35
1:B:195:LYS:HG3	1:B:197:ILE:CD1	1.57	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HB3	1:A:592:PHE:CE2	1.62	1.33
1:C:87:ASN:OD1	1:C:269:TYR:CE2	1.81	1.33
1:B:195:LYS:CG	1:B:197:ILE:HD11	1.58	1.32
1:C:541:PHE:CE2	1:C:587:ILE:HD13	1.64	1.32
1:A:33:THR:HG22	1:A:58:PHE:CD2	1.63	1.31
1:A:823:PHE:O	1:A:827:THR:HG22	1.27	1.31
1:B:543:PHE:CB	1:B:576:VAL:CG2	1.95	1.31
1:A:107:GLY:CA	1:A:235:ILE:HG22	1.61	1.31
1:A:726:ILE:CG2	1:A:948:LEU:HG	1.62	1.30
1:B:426:PRO:CG	1:B:464:PHE:CE1	2.14	1.30
1:B:1104:VAL:CG1	1:B:1119:ASN:ND2	1.94	1.30
1:C:551:VAL:CG1	1:C:590:CYS:SG	2.18	1.30
1:A:64:TRP:CD1	1:A:266:TYR:CD2	2.19	1.29
1:B:1141:LEU:O	1:B:1145:LEU:CD2	1.80	1.29
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	1.46	1.29
1:C:119:ILE:CG1	1:C:128:ILE:HA	1.60	1.29
1:C:490:PHE:CD1	1:C:491:PRO:HD2	1.65	1.29
1:C:541:PHE:CD2	1:C:552:LEU:HD21	1.66	1.29
1:A:784:GLN:OE1	1:A:1030:SER:HB2	1.33	1.28
1:A:743:CYS:SG	1:A:749:CYS:C	2.15	1.27
1:C:118:LEU:HD22	1:C:135:PHE:CZ	1.68	1.26
1:B:1028:LYS:HD3	1:B:1032:CYS:SG	1.74	1.26
1:C:34:ARG:NH1	1:C:221:SER:OG	1.69	1.26
1:A:885:GLY:HA2	1:A:901:GLN:NE2	1.50	1.25
1:B:726:ILE:HG21	1:B:948:LEU:CD1	1.67	1.25
1:C:453:TYR:HD1	1:C:495:TYR:CE1	1.54	1.24
1:A:621:PRO:HB2	1:A:637:SER:OG	1.15	1.24
1:C:541:PHE:CZ	1:C:587:ILE:CD1	2.21	1.24
1:C:330:PRO:HD3	1:C:544:ASN:ND2	1.50	1.24
1:A:204:TYR:CE1	1:A:225:PRO:HB3	1.73	1.23
1:B:353:TRP:CZ3	1:B:466:ARG:CB	2.20	1.23
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	1.53	1.23
1:B:856:ASN:O	1:B:858:LEU:N	1.71	1.23
1:B:521:PRO:HB2	1:B:544:ASN:ND2	1.52	1.23
1:C:453:TYR:CD1	1:C:495:TYR:HE1	1.57	1.22
1:B:515:PHE:C	1:B:516:GLU:OE1	1.81	1.22
1:A:310:LYS:HB2	1:A:600:PRO:O	1.12	1.21
1:C:37:TYR:CE1	1:C:55:PHE:CE1	2.27	1.21
1:A:1021:SER:O	1:A:1025:ALA:N	1.72	1.21
1:B:543:PHE:CD2	1:B:576:VAL:HG13	1.74	1.21
1:B:331:ASN:O	1:B:333:THR:HG23	1.39	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:MET:SD	1:A:1060:VAL:HG11	1.81	1.20
1:C:105:ILE:HG13	1:C:118:LEU:CD1	1.70	1.20
1:A:64:TRP:NE1	1:A:266:TYR:CE2	2.09	1.20
1:B:1088:HIS:CD2	1:B:1137:VAL:HG11	1.76	1.20
1:B:329:PHE:CA	1:B:579:PRO:HG2	1.72	1.20
1:A:823:PHE:O	1:A:827:THR:CG2	1.88	1.19
1:B:726:ILE:CG2	1:B:948:LEU:HD11	1.70	1.19
1:C:119:ILE:HD11	1:C:128:ILE:CG2	1.72	1.19
1:C:607:GLN:NE2	1:C:674:TYR:OH	1.75	1.19
1:B:394:ASN:ND2	1:C:200:TYR:OH	1.73	1.18
1:A:317:ASN:CB	1:A:592:PHE:CZ	2.24	1.18
1:A:726:ILE:HG22	1:A:948:LEU:CG	1.73	1.18
1:C:289:VAL:HG23	1:C:306:PHE:CE2	1.77	1.18
1:C:392:PHE:HE2	1:C:395:VAL:CG2	1.58	1.17
1:B:470:THR:O	1:B:490:PHE:CE1	1.95	1.17
1:A:89:GLY:HA3	1:A:270:LEU:N	1.59	1.17
1:C:420:ASP:O	1:C:460:ASN:OD1	1.62	1.17
1:B:119:ILE:CG1	1:B:128:ILE:HG12	1.75	1.16
1:B:353:TRP:CH2	1:B:466:ARG:CB	2.28	1.16
1:A:905:ARG:HD3	1:A:1049:LEU:O	1.42	1.16
1:A:497:PHE:CE2	1:A:507:PRO:HB3	1.79	1.16
1:B:718:PHE:CB	1:B:1067:TYR:HE1	1.57	1.15
1:C:365:TYR:OH	1:C:392:PHE:HZ	1.23	1.15
1:B:1104:VAL:HG11	1:B:1119:ASN:ND2	1.54	1.15
1:C:735:SER:HB3	1:C:861:LEU:HD21	1.23	1.15
1:C:972:ALA:CB	1:C:996:LEU:HD11	1.76	1.15
1:A:621:PRO:CG	1:A:637:SER:OG	1.93	1.15
1:B:1141:LEU:CD2	1:B:1145:LEU:HD21	1.77	1.15
1:B:329:PHE:HA	1:B:579:PRO:HG2	1.28	1.14
1:B:541:PHE:HZ	1:B:587:ILE:HG21	1.11	1.14
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.28	1.14
1:C:220:PHE:CZ	1:C:288:ALA:N	2.14	1.14
1:A:133:PHE:CE1	1:A:160:TYR:CE1	2.34	1.14
1:A:552:LEU:HD22	1:A:587:ILE:HD13	1.17	1.14
1:C:83:VAL:HG21	1:C:237:ARG:CZ	1.76	1.14
1:C:462:LYS:HA	1:C:462:LYS:HE2	1.30	1.13
1:C:541:PHE:CE2	1:C:552:LEU:HD21	1.84	1.13
1:C:289:VAL:HG23	1:C:306:PHE:CZ	1.82	1.13
1:A:89:GLY:C	1:A:270:LEU:HD13	1.74	1.13
1:C:33:THR:CA	1:C:58:PHE:CE1	2.15	1.13
1:B:329:PHE:C	1:B:579:PRO:HG2	1.72	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:VAL:HG13	1:B:1119:ASN:HD21	1.00	1.12
1:A:317:ASN:CB	1:A:592:PHE:HZ	1.58	1.12
1:B:372:ALA:HB1	1:B:374:PHE:CE2	1.84	1.12
1:B:816:SER:O	1:B:820:ASP:N	1.82	1.12
1:A:1022:ALA:HA	1:A:1025:ALA:HB3	1.14	1.12
1:A:1022:ALA:O	1:A:1026:ALA:N	1.81	1.12
1:B:546:LEU:CD1	1:B:573:THR:HG21	1.78	1.12
1:C:392:PHE:CE2	1:C:395:VAL:CG2	2.31	1.12
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.13	1.11
1:C:552:LEU:CD2	1:C:587:ILE:HG12	1.80	1.11
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.20	1.11
1:C:615:VAL:HG21	1:C:649:CYS:HB3	1.30	1.11
1:A:53:ASP:O	1:A:55:PHE:CD2	2.04	1.11
1:A:620:VAL:HB	1:A:621:PRO:CD	1.79	1.11
1:B:822:LEU:HD21	1:B:1056:ALA:HB2	1.32	1.11
1:C:552:LEU:HD23	1:C:587:ILE:HG12	1.17	1.11
1:A:33:THR:HG22	1:A:58:PHE:CE2	1.85	1.11
1:A:83:VAL:HG21	1:A:237:ARG:CD	1.80	1.11
1:A:89:GLY:CA	1:A:270:LEU:HD13	1.80	1.11
1:A:118:LEU:HD22	1:A:135:PHE:CZ	1.86	1.11
1:B:470:THR:O	1:B:490:PHE:HE1	1.27	1.11
1:B:823:PHE:O	1:B:827:THR:HG23	1.51	1.11
1:C:87:ASN:OD1	1:C:269:TYR:CD2	2.03	1.11
1:C:119:ILE:CG1	1:C:127:VAL:O	1.99	1.10
1:C:392:PHE:HE2	1:C:395:VAL:HG21	1.10	1.10
1:C:598:ILE:HD11	1:C:666:ILE:HD11	1.18	1.10
1:B:521:PRO:CB	1:B:544:ASN:ND2	2.14	1.10
1:B:336:CYS:HG	1:B:362:VAL:C	1.60	1.10
1:B:564:GLN:HE22	1:B:577:ARG:HD2	1.05	1.10
1:C:1090:PRO:HA	1:C:1120:THR:HG22	1.15	1.10
1:B:821:LEU:HD12	1:B:824:ASN:HB3	1.26	1.10
1:B:1039:ARG:CZ	1:B:1042:PHE:CE2	2.34	1.10
1:B:578:ASP:OD1	1:B:581:THR:OG1	1.70	1.09
1:C:516:GLU:CG	1:C:519:HIS:NE2	2.14	1.09
1:B:543:PHE:CG	1:B:576:VAL:CG1	2.34	1.09
1:B:615:VAL:HG11	1:B:620:VAL:HG12	1.13	1.09
1:B:1141:LEU:O	1:B:1145:LEU:HD23	1.36	1.09
1:C:902:MET:HB3	1:C:916:LEU:HD21	1.25	1.09
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.11	1.09
1:C:119:ILE:HG13	1:C:128:ILE:HA	1.14	1.09
1:C:119:ILE:HD11	1:C:128:ILE:HG23	1.13	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ASN:ND2	1:C:200:TYR:CE2	2.21	1.09
1:B:394:ASN:ND2	1:C:200:TYR:CZ	2.21	1.09
1:B:541:PHE:O	1:B:547:THR:HG23	1.50	1.09
1:B:322:PRO:HG3	1:B:540:ASN:OD1	1.53	1.08
1:B:382:VAL:HG23	1:C:983:ARG:O	1.53	1.08
1:C:551:VAL:HG12	1:C:590:CYS:SG	1.91	1.08
1:B:329:PHE:HA	1:B:579:PRO:CG	1.83	1.08
1:A:64:TRP:CD1	1:A:266:TYR:CE2	2.40	1.08
1:B:743:CYS:SG	1:B:750:SER:N	2.26	1.08
1:C:87:ASN:CG	1:C:269:TYR:CD2	2.31	1.08
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.35	1.08
1:A:308:VAL:O	1:A:602:THR:HG22	1.51	1.08
1:A:453:TYR:CE2	1:A:493:GLN:HG2	1.88	1.08
1:B:795:LYS:O	1:B:797:PHE:CD2	2.05	1.08
1:C:544:ASN:HD21	1:C:579:PRO:HG3	1.18	1.08
1:A:1088:HIS:ND1	1:A:1122:VAL:HG13	1.67	1.07
1:B:119:ILE:HD11	1:B:128:ILE:HG23	1.31	1.07
1:B:334:ASN:O	1:B:362:VAL:N	1.86	1.07
1:B:543:PHE:HB3	1:B:576:VAL:HG22	1.30	1.07
1:C:902:MET:HB3	1:C:916:LEU:CD2	1.84	1.07
1:A:826:VAL:CG2	1:A:945:LEU:HD13	1.84	1.06
1:B:537:LYS:C	1:B:551:VAL:HG12	1.79	1.06
1:B:613:GLN:O	1:B:647:ALA:O	1.72	1.06
1:B:718:PHE:CB	1:B:1067:TYR:CE1	2.32	1.06
1:C:105:ILE:HD11	1:C:241:LEU:CD1	1.84	1.06
1:A:37:TYR:OH	1:A:195:LYS:NZ	1.88	1.06
1:A:83:VAL:HG21	1:A:237:ARG:HD2	1.08	1.06
1:A:105:ILE:HG13	1:A:118:LEU:HD13	1.31	1.06
1:B:1028:LYS:CD	1:B:1032:CYS:SG	2.41	1.06
1:C:210:ILE:HB	1:C:212:LEU:HD21	1.36	1.06
1:C:825:LYS:NZ	1:C:942:ALA:HB2	1.70	1.06
1:B:329:PHE:CD2	1:B:330:PRO:HD2	1.88	1.06
1:B:521:PRO:HB2	1:B:544:ASN:HD21	0.89	1.06
1:C:662:CYS:SG	1:C:697:MET:HB3	1.96	1.06
1:B:543:PHE:HB2	1:B:576:VAL:HG21	1.08	1.05
1:C:598:ILE:CD1	1:C:666:ILE:HD11	1.87	1.05
1:B:57:PRO:HB3	1:B:273:ARG:HH12	1.04	1.05
1:B:322:PRO:HG3	1:B:549:THR:HG21	1.31	1.05
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.31	1.05
1:A:726:ILE:HD12	1:A:944:ALA:O	1.55	1.05
1:B:298:GLU:HG2	1:B:315:THR:HG21	1.39	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:HE1	1:C:55:PHE:CE1	1.70	1.05
1:C:972:ALA:HB2	1:C:996:LEU:HD11	1.34	1.05
1:C:55:PHE:HD2	1:C:275:PHE:CD1	1.75	1.05
1:A:639:GLY:HA3	1:A:642:VAL:CG2	1.86	1.04
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.39	1.04
1:B:197:ILE:HB	1:B:202:LYS:HE3	1.34	1.04
1:B:1141:LEU:HD23	1:B:1145:LEU:HD21	1.38	1.04
1:C:1102:TRP:HB2	1:C:1135:ASN:OD1	1.57	1.04
1:B:336:CYS:SG	1:B:362:VAL:C	2.40	1.04
1:A:90:VAL:HG23	1:A:238:PHE:CE2	1.91	1.04
1:B:546:LEU:HD13	1:B:573:THR:HG21	1.04	1.04
1:B:985:ASP:O	1:B:989:ALA:CB	2.05	1.04
1:C:200:TYR:HD2	1:C:230:PRO:HA	1.17	1.04
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.36	1.04
1:A:319:ARG:HG2	1:A:592:PHE:HD2	1.19	1.04
1:B:576:VAL:HG12	1:B:587:ILE:HD11	1.37	1.04
1:B:638:THR:O	1:B:642:VAL:HG12	1.57	1.04
1:C:615:VAL:HG23	1:C:649:CYS:HB2	1.39	1.04
1:C:1089:PHE:O	1:C:1120:THR:HB	1.56	1.04
1:A:89:GLY:O	1:A:269:TYR:HA	1.59	1.03
1:A:89:GLY:HA2	1:A:270:LEU:HD13	1.40	1.03
1:A:299:THR:OG1	1:A:597:VAL:HG21	1.57	1.03
1:B:197:ILE:HD13	1:B:202:LYS:HD2	1.37	1.03
1:C:551:VAL:HG11	1:C:590:CYS:SG	1.98	1.03
1:A:620:VAL:HG23	1:A:621:PRO:HD2	1.37	1.03
1:C:763:LEU:HD13	1:C:1004:LEU:CD2	1.87	1.03
1:B:541:PHE:CZ	1:B:587:ILE:HD13	1.93	1.03
1:A:278:LYS:HB2	1:A:306:PHE:CE2	1.94	1.03
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.27	1.03
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	0.90	1.03
1:B:118:LEU:HD22	1:B:135:PHE:CE1	1.94	1.02
1:C:200:TYR:CD2	1:C:230:PRO:HA	1.92	1.02
1:C:337:PRO:HD2	1:C:358:ILE:HD11	1.36	1.02
1:C:736:VAL:CG2	1:C:858:LEU:HD12	1.90	1.02
1:A:83:VAL:CG2	1:A:237:ARG:HD2	1.89	1.02
1:A:310:LYS:CB	1:A:600:PRO:O	2.06	1.02
1:B:118:LEU:HD22	1:B:135:PHE:CZ	1.95	1.02
1:C:392:PHE:CE2	1:C:395:VAL:HG21	1.91	1.02
1:A:784:GLN:CD	1:A:1030:SER:HB2	1.84	1.02
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.23	1.02
1:A:1088:HIS:ND1	1:A:1122:VAL:CG1	2.23	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.24	1.01
1:A:559:PHE:HE1	1:A:584:ILE:HB	1.24	1.01
1:C:472:ILE:HG22	1:C:490:PHE:HA	1.39	1.01
1:C:735:SER:CB	1:C:861:LEU:HD21	1.89	1.01
1:C:1087:ALA:O	1:C:1122:VAL:HG23	1.60	1.01
1:C:502:GLY:O	1:C:506:GLN:HG3	1.59	1.01
1:B:543:PHE:CD2	1:B:576:VAL:CG1	2.44	1.00
1:C:392:PHE:CE2	1:C:395:VAL:HG22	1.95	1.00
1:C:119:ILE:CG1	1:C:128:ILE:CA	2.39	1.00
1:A:89:GLY:CA	1:A:270:LEU:CD1	2.38	1.00
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.43	1.00
1:B:328:ARG:CZ	1:B:578:ASP:OD2	2.10	1.00
1:B:393:THR:HG23	1:B:522:ALA:HB2	1.41	1.00
1:A:784:GLN:OE1	1:A:1030:SER:CB	2.10	1.00
1:B:543:PHE:CG	1:B:576:VAL:HG11	1.94	1.00
1:B:201:PHE:HE1	1:B:203:ILE:HG13	1.26	1.00
1:C:118:LEU:CD2	1:C:135:PHE:CZ	2.43	1.00
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.42	1.00
1:B:1104:VAL:HG13	1:B:1119:ASN:ND2	1.67	1.00
1:B:699:LEU:HD23	1:C:788:ILE:HG13	1.44	0.99
1:C:36:VAL:O	1:C:223:LEU:CD2	2.10	0.99
1:C:119:ILE:HD11	1:C:128:ILE:CB	1.92	0.99
1:A:83:VAL:CG2	1:A:237:ARG:CD	2.40	0.99
1:B:1010:GLN:CB	1:B:1014:ARG:HH12	1.75	0.99
1:C:736:VAL:HG23	1:C:858:LEU:HD12	1.44	0.99
1:C:825:LYS:HZ1	1:C:942:ALA:HB2	1.19	0.99
1:C:85:PRO:HG2	1:C:269:TYR:OH	1.63	0.99
1:A:353:TRP:CG	1:A:466:ARG:HD3	1.95	0.99
1:B:126:VAL:HG13	1:B:175:PHE:CE1	1.96	0.99
1:B:718:PHE:CD2	1:B:1067:TYR:CE1	2.50	0.99
1:C:89:GLY:C	1:C:270:LEU:HD13	1.87	0.99
1:B:328:ARG:NH1	1:B:578:ASP:OD2	1.96	0.99
1:B:322:PRO:CG	1:B:549:THR:HG21	1.92	0.98
1:C:105:ILE:CG1	1:C:118:LEU:HD13	1.92	0.98
1:A:621:PRO:CB	1:A:637:SER:HG	1.61	0.98
1:B:396:TYR:HE2	1:C:200:TYR:HH	0.99	0.98
1:B:541:PHE:CZ	1:B:587:ILE:HG21	1.98	0.98
1:C:977:LEU:HD11	1:C:1000:ARG:HH12	1.27	0.98
1:C:1010:GLN:OE1	1:C:1014:ARG:NH1	1.97	0.98
1:B:342:PHE:HE2	1:B:368:LEU:CD1	1.76	0.98
1:B:577:ARG:HD3	1:B:582:LEU:HD23	1.43	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:CG	1:C:269:TYR:HD2	1.68	0.98
1:A:89:GLY:C	1:A:270:LEU:CD1	2.37	0.97
1:B:1088:HIS:CE1	1:B:1122:VAL:HG23	1.99	0.97
1:C:453:TYR:CD1	1:C:495:TYR:CE1	2.40	0.97
1:B:85:PRO:O	1:B:269:TYR:OH	1.80	0.97
1:C:119:ILE:CD1	1:C:128:ILE:HG23	1.93	0.97
1:B:726:ILE:HG21	1:B:948:LEU:HD11	1.33	0.97
1:B:1081:ILE:O	1:B:1088:HIS:HB2	1.64	0.97
1:C:615:VAL:CG2	1:C:649:CYS:CB	2.41	0.97
1:B:119:ILE:HG12	1:B:128:ILE:CG1	1.94	0.97
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.46	0.97
1:A:726:ILE:CG2	1:A:948:LEU:CG	2.36	0.97
1:B:718:PHE:CG	1:B:1067:TYR:HE1	1.82	0.97
1:A:353:TRP:H	1:A:466:ARG:HD2	1.29	0.97
1:B:543:PHE:CD1	1:B:576:VAL:HG11	1.99	0.97
1:C:727:LEU:HD11	1:C:1028:LYS:HZ2	1.28	0.97
1:A:1102:TRP:HB2	1:A:1135:ASN:HD21	1.05	0.97
1:B:126:VAL:HG22	1:B:172:SER:HB3	1.43	0.97
1:B:322:PRO:HG3	1:B:549:THR:CG2	1.94	0.97
1:C:612:TYR:O	1:C:615:VAL:HG22	1.65	0.97
1:A:592:PHE:CD1	1:A:593:GLY:N	2.32	0.97
1:B:331:ASN:O	1:B:332:ILE:C	2.04	0.97
1:C:33:THR:HA	1:C:58:PHE:CD1	1.98	0.97
1:A:715:PRO:HA	1:A:1071:GLN:O	1.65	0.97
1:A:781:VAL:CG1	1:A:1029:MET:HG3	1.94	0.97
1:B:201:PHE:CE1	1:B:203:ILE:HG13	2.00	0.96
1:B:638:THR:O	1:B:642:VAL:CG1	2.13	0.96
1:C:37:TYR:CD1	1:C:55:PHE:HE1	1.82	0.96
1:A:33:THR:CG2	1:A:58:PHE:CE2	2.47	0.96
1:A:521:PRO:HG3	1:A:564:GLN:HG3	1.47	0.96
1:A:797:PHE:CE1	1:A:882:ILE:HG21	1.99	0.96
1:B:106:PHE:HB3	1:B:235:ILE:CD1	1.96	0.96
1:B:1039:ARG:NH1	1:B:1042:PHE:CE2	2.33	0.96
1:B:92:PHE:CZ	1:B:265:TYR:HD2	1.83	0.96
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.46	0.96
1:C:220:PHE:CE2	1:C:288:ALA:N	2.33	0.96
1:C:377:PHE:CD1	1:C:434:ILE:HG13	2.00	0.96
1:B:961:THR:O	1:B:965:GLN:HG2	1.66	0.96
1:A:781:VAL:HG12	1:A:1029:MET:HG3	1.43	0.96
1:C:186:PHE:O	1:C:211:ASN:HB3	1.65	0.96
1:C:318:PHE:CD1	1:C:593:GLY:HA3	2.00	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:PHE:HE1	1:C:431:GLY:O	1.48	0.96
1:C:426:PRO:HG2	1:C:464:PHE:CE2	2.00	0.96
1:A:87:ASN:ND2	1:A:269:TYR:CD1	2.34	0.95
1:A:107:GLY:N	1:A:235:ILE:HG22	1.79	0.95
1:B:615:VAL:CG1	1:B:620:VAL:HG12	1.96	0.95
1:C:220:PHE:CE2	1:C:287:ASP:HA	2.01	0.95
1:B:521:PRO:CB	1:B:544:ASN:HD21	1.77	0.95
1:C:544:ASN:ND2	1:C:579:PRO:HG3	1.80	0.95
1:B:615:VAL:HG11	1:B:620:VAL:CG1	1.96	0.95
1:C:598:ILE:HD11	1:C:666:ILE:HD12	1.48	0.95
1:C:825:LYS:CE	1:C:942:ALA:HB2	1.97	0.95
1:A:620:VAL:CG2	1:A:621:PRO:HD2	1.95	0.95
1:B:1028:LYS:NZ	1:B:1042:PHE:O	1.98	0.95
1:C:615:VAL:CG2	1:C:649:CYS:HB3	1.96	0.95
1:B:823:PHE:HA	1:B:826:VAL:CG1	1.97	0.94
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	1.63	0.94
1:C:1095:PHE:CZ	1:C:1120:THR:HG21	2.02	0.94
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	1.83	0.94
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	1.80	0.94
1:B:1141:LEU:HD23	1:B:1145:LEU:CD2	1.97	0.94
1:A:620:VAL:CB	1:A:621:PRO:CD	2.44	0.94
1:A:133:PHE:CD1	1:A:160:TYR:CD1	2.55	0.94
1:A:353:TRP:CD1	1:A:466:ARG:HD3	2.01	0.94
1:B:57:PRO:CB	1:B:273:ARG:HH12	1.80	0.94
1:C:37:TYR:CE1	1:C:55:PHE:HE1	1.73	0.94
1:C:289:VAL:CG2	1:C:306:PHE:CE2	2.50	0.94
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.00	0.94
1:C:429:PHE:CZ	1:C:431:GLY:HA3	2.01	0.94
1:A:541:PHE:CE2	1:A:587:ILE:HD12	2.01	0.94
1:B:544:ASN:O	1:B:565:PHE:CZ	2.20	0.94
1:C:119:ILE:CD1	1:C:128:ILE:HA	1.97	0.94
1:C:119:ILE:HG23	1:C:127:VAL:O	1.68	0.94
1:C:615:VAL:HG23	1:C:649:CYS:CB	1.97	0.94
1:B:1039:ARG:CZ	1:B:1042:PHE:CD2	2.51	0.94
1:A:743:CYS:SG	1:A:750:SER:N	2.41	0.93
1:A:204:TYR:HE1	1:A:225:PRO:HB3	1.14	0.93
1:B:360:ASN:OD1	1:B:523:THR:CG2	2.17	0.93
1:B:1088:HIS:HD2	1:B:1137:VAL:HG11	1.23	0.93
1:C:330:PRO:CD	1:C:544:ASN:ND2	2.31	0.93
1:A:204:TYR:CD1	1:A:225:PRO:HA	2.04	0.93
1:A:639:GLY:HA3	1:A:642:VAL:HG23	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PHE:HE2	1:B:368:LEU:HD12	1.34	0.93
1:B:617:CYS:N	1:B:649:CYS:SG	2.41	0.93
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	1.49	0.93
1:B:543:PHE:CE2	1:B:576:VAL:HG13	2.02	0.93
1:B:544:ASN:O	1:B:565:PHE:HZ	1.50	0.93
1:B:1028:LYS:HZ3	1:B:1042:PHE:HD1	1.09	0.93
1:C:671:CYS:SG	1:C:697:MET:HB3	2.09	0.93
1:B:472:ILE:HG23	1:B:489:TYR:O	1.69	0.93
1:B:541:PHE:CE1	1:B:587:ILE:HD13	2.03	0.93
1:B:784:GLN:HA	1:B:784:GLN:HE21	1.29	0.93
1:C:83:VAL:HG21	1:C:237:ARG:NH2	1.84	0.93
1:B:599:THR:HG22	1:B:608:VAL:CG1	1.99	0.93
1:B:317:ASN:HD22	1:C:737:ASP:CG	1.77	0.92
1:C:392:PHE:CD2	1:C:395:VAL:HG22	2.02	0.92
1:A:89:GLY:CA	1:A:270:LEU:HB2	1.99	0.92
1:A:85:PRO:HG2	1:A:269:TYR:OH	1.69	0.92
1:C:374:PHE:HD2	1:C:436:TRP:CD1	1.88	0.92
1:C:905:ARG:HD2	1:C:1049:LEU:O	1.69	0.92
1:A:621:PRO:HG2	1:A:637:SER:OG	1.67	0.92
1:A:724:THR:HG22	1:A:1063:LEU:HD23	1.51	0.92
1:C:392:PHE:CE2	1:C:524:VAL:HG11	2.05	0.92
1:B:546:LEU:HD13	1:B:573:THR:CG2	1.98	0.92
1:C:36:VAL:O	1:C:223:LEU:HD21	1.69	0.92
1:A:107:GLY:HA2	1:A:235:ILE:HG22	1.46	0.92
1:B:426:PRO:HG3	1:B:464:PHE:CE1	2.04	0.92
1:C:105:ILE:CG1	1:C:118:LEU:CD1	2.46	0.92
1:A:324:GLU:O	1:A:539:VAL:HB	1.68	0.92
1:B:298:GLU:CG	1:B:315:THR:HG21	1.99	0.92
1:B:342:PHE:CE2	1:B:368:LEU:CD1	2.53	0.92
1:A:826:VAL:HG22	1:A:945:LEU:HD13	1.49	0.91
1:B:1090:PRO:CB	1:B:1093:GLY:O	2.17	0.91
1:C:119:ILE:CG1	1:C:128:ILE:HG12	2.00	0.91
1:C:734:THR:O	1:C:767:LEU:HD12	1.70	0.91
1:A:107:GLY:N	1:A:235:ILE:CG2	2.33	0.91
1:B:718:PHE:CD2	1:B:1067:TYR:HE1	1.86	0.91
1:A:552:LEU:HD22	1:A:587:ILE:CD1	2.01	0.91
1:C:105:ILE:HG13	1:C:118:LEU:HD13	1.51	0.91
1:A:96:GLU:OE1	1:A:101:ILE:N	2.03	0.91
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.31	0.91
1:B:480:CYS:O	1:B:483:VAL:HG12	1.70	0.91
1:B:331:ASN:O	1:B:333:THR:N	2.04	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:CYS:HG	1:C:166:CYS:HG	1.02	0.91
1:C:186:PHE:O	1:C:211:ASN:CB	2.18	0.91
1:C:87:ASN:OD1	1:C:269:TYR:HE2	1.33	0.91
1:C:516:GLU:HG3	1:C:519:HIS:CD2	2.05	0.91
1:C:763:LEU:CD1	1:C:1004:LEU:HD22	2.00	0.91
1:A:133:PHE:CE1	1:A:160:TYR:CD1	2.58	0.90
1:B:826:VAL:HG21	1:B:1057:PRO:HG3	1.52	0.90
1:C:655:HIS:HB2	1:C:694:ALA:O	1.70	0.90
1:A:64:TRP:HD1	1:A:266:TYR:CD2	1.74	0.90
1:A:353:TRP:H	1:A:466:ARG:CD	1.84	0.90
1:B:540:ASN:HA	1:B:549:THR:HA	1.54	0.90
1:B:96:GLU:OE1	1:B:101:ILE:N	2.03	0.90
1:C:541:PHE:CE1	1:C:587:ILE:HD13	2.07	0.90
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ3	1.33	0.90
1:B:564:GLN:NE2	1:B:577:ARG:HD2	1.87	0.90
1:B:1039:ARG:CZ	1:B:1042:PHE:HE2	1.85	0.90
1:C:969:ASN:OD1	1:C:975:SER:HB3	1.70	0.90
1:A:53:ASP:O	1:A:55:PHE:CE2	2.24	0.90
1:A:328:ARG:HD3	1:A:531:THR:O	1.71	0.90
1:B:662:CYS:HG	1:B:671:CYS:HG	0.98	0.90
1:B:1141:LEU:O	1:B:1145:LEU:HD22	1.72	0.89
1:C:392:PHE:O	1:C:524:VAL:HB	1.72	0.89
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.86	0.89
1:B:1079:PRO:HG2	1:B:1131:GLY:O	1.72	0.89
1:C:977:LEU:HG	1:C:1000:ARG:HH22	1.35	0.89
1:A:1096:VAL:HG21	1:A:1105:THR:HG22	1.53	0.89
1:C:119:ILE:HG12	1:C:128:ILE:CG1	2.01	0.89
1:B:56:LEU:HD12	1:B:57:PRO:CD	2.02	0.89
1:A:34:ARG:NH1	1:A:217:PRO:HG2	1.88	0.89
1:A:452:LEU:HD13	1:A:493:GLN:O	1.72	0.89
1:B:578:ASP:CG	1:B:581:THR:OG1	2.15	0.89
1:B:1011:GLN:HE21	1:B:1011:GLN:HA	1.34	0.89
1:C:273:ARG:NH1	1:C:292:ALA:HB3	1.88	0.89
1:A:90:VAL:CG1	1:A:194:PHE:HB2	2.02	0.89
1:A:322:PRO:HG2	1:A:540:ASN:OD1	1.72	0.89
1:B:516:GLU:OE1	1:B:516:GLU:N	2.04	0.89
1:B:119:ILE:HG13	1:B:128:ILE:HA	1.54	0.89
1:B:454:ARG:HA	1:B:491:PRO:O	1.73	0.89
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.54	0.89
1:C:612:TYR:HB2	1:C:615:VAL:CG1	2.03	0.89
1:A:984:LEU:CD1	1:A:988:GLU:HG3	2.02	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TYR:HB3	1:B:387:LEU:HD12	1.53	0.88
1:B:722:VAL:CG1	1:B:934:ILE:HG13	2.03	0.88
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.34	0.88
1:C:350:VAL:CG1	1:C:422:ASN:HB3	2.02	0.88
1:A:107:GLY:C	1:A:235:ILE:HG22	1.98	0.88
1:B:1140:PRO:O	1:B:1143:PRO:HD2	1.73	0.88
1:C:102:ARG:HD2	1:C:141:LEU:HD13	1.55	0.88
1:C:977:LEU:CD1	1:C:1000:ARG:HH12	1.85	0.88
1:A:906:PHE:O	1:A:909:ILE:HG12	1.73	0.88
1:C:220:PHE:HZ	1:C:288:ALA:N	1.70	0.88
1:A:204:TYR:CE1	1:A:225:PRO:CB	2.56	0.88
1:B:85:PRO:HG2	1:B:269:TYR:OH	1.74	0.88
1:B:152:TRP:CH2	1:B:245:HIS:CE1	2.61	0.88
1:B:201:PHE:HE1	1:B:203:ILE:CG1	1.87	0.88
1:A:1087:ALA:HB2	1:A:1126:CYS:HB3	1.52	0.88
1:B:821:LEU:HD12	1:B:824:ASN:CB	2.03	0.88
1:B:1095:PHE:CZ	1:B:1120:THR:HG21	2.09	0.88
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.38	0.88
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.47	0.88
1:A:105:ILE:HG13	1:A:118:LEU:CD1	2.03	0.88
1:B:541:PHE:O	1:B:547:THR:CG2	2.20	0.88
1:A:83:VAL:HG22	1:A:237:ARG:HD3	1.55	0.88
1:A:729:VAL:HG21	1:A:1060:VAL:HG23	1.56	0.88
1:B:298:GLU:HG2	1:B:315:THR:CG2	2.03	0.88
1:B:718:PHE:HD2	1:B:1067:TYR:CE1	1.88	0.88
1:A:985:ASP:OD1	1:A:986:PRO:HD2	1.73	0.88
1:B:322:PRO:CG	1:B:540:ASN:OD1	2.22	0.88
1:B:538:CYS:N	1:B:551:VAL:HG12	1.87	0.88
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.56	0.87
1:B:1080:ALA:HB2	1:B:1089:PHE:CE1	2.09	0.87
1:C:429:PHE:CE1	1:C:431:GLY:N	2.42	0.87
1:A:101:ILE:HD11	1:A:263:ALA:HB1	1.55	0.87
1:B:353:TRP:HZ3	1:B:466:ARG:HB2	1.35	0.87
1:C:360:ASN:HD22	1:C:523:THR:HG21	1.35	0.87
1:C:490:PHE:CG	1:C:491:PRO:HD2	2.09	0.87
1:A:559:PHE:CE1	1:A:584:ILE:HB	2.09	0.87
1:B:200:TYR:OH	1:B:202:LYS:HE2	1.74	0.87
1:B:533:LEU:HD12	1:B:534:VAL:N	1.88	0.87
1:C:541:PHE:CE2	1:C:587:ILE:HG21	2.10	0.87
1:C:1095:PHE:HZ	1:C:1120:THR:HG21	1.35	0.87
1:B:726:ILE:CG2	1:B:948:LEU:CD1	2.38	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:VAL:HA	1:C:506:GLN:CD	1.99	0.87
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.39	0.87
1:B:195:LYS:HG3	1:B:197:ILE:HD11	0.87	0.87
1:B:329:PHE:HD2	1:B:330:PRO:HD2	1.39	0.87
1:C:55:PHE:CD2	1:C:275:PHE:CD1	2.61	0.87
1:C:366:SER:O	1:C:370:ASN:N	2.06	0.87
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.08	0.86
1:B:328:ARG:O	1:B:579:PRO:HD2	1.75	0.86
1:B:959:LEU:O	1:B:963:VAL:HG23	1.75	0.86
1:C:119:ILE:CG2	1:C:127:VAL:O	2.22	0.86
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.57	0.86
1:B:541:PHE:CZ	1:B:587:ILE:CG2	2.58	0.86
1:C:119:ILE:HG13	1:C:128:ILE:CA	2.01	0.86
1:C:541:PHE:CE2	1:C:587:ILE:CD1	2.50	0.86
1:A:976:VAL:HG13	1:A:979:ASP:HB3	1.54	0.86
1:C:972:ALA:HB1	1:C:996:LEU:HD11	1.55	0.86
1:A:726:ILE:HG22	1:A:948:LEU:HG	0.87	0.86
1:C:972:ALA:HB2	1:C:996:LEU:CD1	2.05	0.86
1:A:89:GLY:HA3	1:A:270:LEU:CA	2.05	0.86
1:A:731:MET:HG2	1:A:774:GLN:OE1	1.76	0.86
1:B:197:ILE:HD13	1:B:202:LYS:CD	2.05	0.86
1:B:541:PHE:C	1:B:547:THR:HG23	1.99	0.86
1:C:471:GLU:O	1:C:491:PRO:HB3	1.76	0.86
1:B:200:TYR:CZ	1:B:202:LYS:HE2	2.11	0.86
1:B:733:LYS:HD3	1:B:775:ASP:OD1	1.76	0.86
1:B:119:ILE:HD11	1:B:128:ILE:CG2	2.06	0.85
1:C:821:LEU:HD21	1:C:939:SER:HB3	1.57	0.85
1:B:540:ASN:OD1	1:B:549:THR:CG2	2.24	0.85
1:B:543:PHE:CZ	1:B:585:LEU:HD12	2.10	0.85
1:B:541:PHE:HZ	1:B:587:ILE:CG2	1.90	0.85
1:C:105:ILE:HG21	1:C:135:PHE:HE2	1.40	0.85
1:A:89:GLY:HA3	1:A:270:LEU:CB	2.06	0.85
1:A:104:TRP:O	1:A:118:LEU:HD12	1.76	0.85
1:A:805:ILE:O	1:A:816:SER:OG	1.93	0.85
1:B:718:PHE:HB2	1:B:1067:TYR:CZ	2.11	0.85
1:B:722:VAL:O	1:B:934:ILE:HD11	1.77	0.85
1:A:826:VAL:HG11	1:A:1057:PRO:HG2	1.59	0.85
1:A:1102:TRP:CB	1:A:1135:ASN:ND2	2.39	0.85
1:B:91:TYR:CE1	1:B:93:ALA:HB2	2.10	0.85
1:B:1141:LEU:CG	1:B:1145:LEU:HD21	2.07	0.85
1:C:220:PHE:HZ	1:C:288:ALA:CA	1.89	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.57	0.85
1:A:639:GLY:HA3	1:A:642:VAL:HG22	1.56	0.85
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.12	0.85
1:C:429:PHE:CZ	1:C:431:GLY:CA	2.59	0.85
1:A:89:GLY:HA3	1:A:270:LEU:H	1.33	0.85
1:A:726:ILE:CG2	1:A:948:LEU:CD1	2.54	0.85
1:A:1080:ALA:O	1:A:1132:ILE:HG13	1.76	0.85
1:B:190:ARG:HE	1:B:207:HIS:HE1	1.20	0.85
1:B:365:TYR:CE1	1:B:387:LEU:HB3	2.12	0.85
1:B:426:PRO:CG	1:B:464:PHE:CZ	2.44	0.85
1:A:55:PHE:HB3	1:A:275:PHE:CE2	2.12	0.84
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.57	0.84
1:B:336:CYS:SG	1:B:362:VAL:O	2.33	0.84
1:C:102:ARG:CD	1:C:141:LEU:HD13	2.07	0.84
1:A:621:PRO:HB2	1:A:637:SER:HG	0.75	0.84
1:B:328:ARG:C	1:B:579:PRO:HD2	2.02	0.84
1:C:366:SER:O	1:C:370:ASN:CB	2.25	0.84
1:A:826:VAL:HG23	1:A:945:LEU:HD13	1.57	0.84
1:A:331:ASN:CG	1:A:580:GLN:NE2	2.35	0.84
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.36	0.84
1:C:220:PHE:HZ	1:C:288:ALA:CB	1.89	0.84
1:C:490:PHE:CD1	1:C:491:PRO:CD	2.58	0.84
1:A:317:ASN:CB	1:A:592:PHE:CE2	2.54	0.84
1:A:331:ASN:H	1:A:580:GLN:NE2	1.75	0.84
1:C:429:PHE:CE1	1:C:431:GLY:CA	2.60	0.84
1:C:33:THR:HG22	1:C:58:PHE:CE1	2.13	0.84
1:C:986:PRO:O	1:C:990:GLU:HG2	1.76	0.84
1:B:294:ASP:HB2	1:B:297:SER:OG	1.76	0.84
1:B:822:LEU:O	1:B:826:VAL:HG12	1.77	0.84
1:B:335:LEU:O	1:B:361:CYS:HB2	1.76	0.84
1:B:1114:ILE:HG23	1:B:1138:TYR:CE1	2.12	0.84
1:C:598:ILE:CD1	1:C:666:ILE:CD1	2.48	0.84
1:A:89:GLY:CA	1:A:270:LEU:CB	2.56	0.84
1:B:44:ARG:HB3	1:B:47:VAL:CG2	2.06	0.84
1:B:718:PHE:HZ	1:B:923:ILE:HD11	1.42	0.84
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.59	0.84
1:C:105:ILE:HD11	1:C:241:LEU:HD11	1.58	0.84
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.59	0.84
1:C:552:LEU:CD2	1:C:587:ILE:CG1	2.55	0.84
1:C:290:ASP:O	1:C:297:SER:HB3	1.78	0.84
1:C:731:MET:O	1:C:774:GLN:HG3	1.78	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.13	0.83
1:C:1090:PRO:CA	1:C:1120:THR:HG22	2.06	0.83
1:A:420:ASP:HB3	1:A:460:ASN:OD1	1.78	0.83
1:C:33:THR:CB	1:C:58:PHE:HE1	1.91	0.83
1:C:87:ASN:ND2	1:C:269:TYR:CD2	2.45	0.83
1:B:576:VAL:CG1	1:B:587:ILE:HD11	2.07	0.83
1:C:210:ILE:HB	1:C:212:LEU:CD2	2.07	0.83
1:C:32:PHE:CE1	1:C:218:GLN:HB3	2.13	0.83
1:B:1090:PRO:HB2	1:B:1093:GLY:O	1.78	0.83
1:C:119:ILE:HG13	1:C:127:VAL:O	1.76	0.83
1:A:1022:ALA:CA	1:A:1025:ALA:HB3	2.03	0.83
1:B:126:VAL:CG2	1:B:172:SER:CB	2.56	0.83
1:A:241:LEU:HD12	1:A:242:LEU:N	1.94	0.83
1:A:331:ASN:H	1:A:580:GLN:HE22	1.22	0.83
1:A:897:PRO:HG2	1:A:900:MET:SD	2.19	0.83
1:B:200:TYR:HB2	1:B:230:PRO:HA	1.59	0.83
1:B:331:ASN:O	1:B:333:THR:CG2	2.25	0.83
1:B:426:PRO:HG3	1:B:464:PHE:CD1	2.12	0.83
1:B:485:GLY:O	1:B:488:CYS:HB2	1.77	0.83
1:B:770:ILE:HD11	1:B:1012:LEU:HD12	1.61	0.83
1:C:756:TYR:HB3	1:C:759:PHE:CD2	2.13	0.83
1:A:89:GLY:HA2	1:A:270:LEU:CD1	2.05	0.83
1:B:726:ILE:HG22	1:B:948:LEU:HD11	1.61	0.83
1:C:727:LEU:HD11	1:C:1028:LYS:NZ	1.94	0.83
1:C:1081:ILE:O	1:C:1088:HIS:HB2	1.79	0.83
1:A:204:TYR:HD1	1:A:225:PRO:CA	1.92	0.83
1:B:324:GLU:O	1:B:539:VAL:CG2	2.27	0.83
1:A:204:TYR:CD1	1:A:225:PRO:CA	2.62	0.82
1:A:611:LEU:HB2	1:A:650:LEU:HD22	1.58	0.82
1:B:342:PHE:CE2	1:B:368:LEU:HD11	2.14	0.82
1:A:91:TYR:HD1	1:A:193:VAL:HG22	1.43	0.82
1:A:353:TRP:HZ2	1:A:465:GLU:C	1.87	0.82
1:A:453:TYR:CE2	1:A:493:GLN:CG	2.62	0.82
1:B:107:GLY:N	1:B:235:ILE:HD13	1.95	0.82
1:B:472:ILE:CD1	1:B:490:PHE:HB2	2.09	0.82
1:B:856:ASN:C	1:B:858:LEU:H	1.88	0.82
1:B:1090:PRO:HA	1:B:1120:THR:HG22	1.61	0.82
1:A:319:ARG:CG	1:A:592:PHE:HD2	1.91	0.82
1:B:1039:ARG:NH2	1:B:1042:PHE:HE2	1.77	0.82
1:A:317:ASN:HB3	1:A:592:PHE:HZ	1.02	0.82
1:C:350:VAL:HG12	1:C:422:ASN:CB	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:PHE:CE1	1:A:882:ILE:CG2	2.62	0.82
1:A:673:SER:O	1:A:693:ILE:HD13	1.79	0.82
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.47	0.82
1:A:43:PHE:HE2	1:A:282:ASN:O	1.62	0.82
1:B:44:ARG:HB2	1:B:279:TYR:CD2	2.15	0.82
1:B:574:ASP:O	1:B:587:ILE:HB	1.79	0.82
1:B:540:ASN:OD1	1:B:549:THR:OG1	1.97	0.82
1:B:546:LEU:CD1	1:B:573:THR:CG2	2.58	0.82
1:C:380:TYR:CE2	1:C:412:PRO:CD	2.63	0.82
1:C:662:CYS:SG	1:C:697:MET:CB	2.68	0.81
1:B:715:PRO:HA	1:B:1071:GLN:O	1.80	0.81
1:B:1090:PRO:HD3	1:B:1095:PHE:HE1	1.44	0.81
1:A:204:TYR:HE1	1:A:225:PRO:CB	1.91	0.81
1:C:105:ILE:CG2	1:C:118:LEU:HD13	2.10	0.81
1:C:119:ILE:CB	1:C:127:VAL:O	2.27	0.81
1:C:957:GLN:O	1:C:961:THR:OG1	1.96	0.81
1:A:89:GLY:HA2	1:A:270:LEU:HB2	1.62	0.81
1:A:516:GLU:N	1:A:516:GLU:OE1	2.14	0.81
1:B:89:GLY:C	1:B:270:LEU:CD1	2.53	0.81
1:B:797:PHE:HB2	1:B:800:PHE:O	1.81	0.81
1:C:458:LYS:N	1:C:473:TYR:HE1	1.79	0.81
1:C:495:TYR:HD2	1:C:497:PHE:HE2	1.25	0.81
1:A:107:GLY:CA	1:A:235:ILE:CG2	2.52	0.81
1:C:119:ILE:HG12	1:C:127:VAL:O	1.81	0.81
1:A:33:THR:CB	1:A:58:PHE:CE2	2.64	0.81
1:A:319:ARG:HG2	1:A:592:PHE:CD2	2.11	0.81
1:B:564:GLN:HE22	1:B:577:ARG:CD	1.91	0.81
1:B:1116:THR:HG22	1:B:1140:PRO:HD3	1.63	0.81
1:C:105:ILE:HG23	1:C:118:LEU:HD13	1.62	0.81
1:A:817:PHE:HE2	1:A:935:GLN:HG3	1.46	0.81
1:A:1090:PRO:CB	1:A:1093:GLY:O	2.28	0.81
1:B:394:ASN:ND2	1:C:200:TYR:HE2	1.78	0.81
1:B:1104:VAL:CG1	1:B:1119:ASN:HD22	1.85	0.81
1:C:856:ASN:OD1	1:C:966:LEU:HD13	1.80	0.81
1:B:902:MET:HB3	1:B:916:LEU:HD21	1.63	0.81
1:C:220:PHE:CZ	1:C:288:ALA:CB	2.64	0.81
1:C:581:THR:HG22	1:C:583:GLU:HG3	1.63	0.81
1:C:1014:ARG:O	1:C:1018:ILE:HG12	1.81	0.81
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.16	0.80
1:B:275:PHE:CD1	1:B:290:ASP:HA	2.15	0.80
1:A:350:VAL:HG12	1:A:452:LEU:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.16	0.80
1:B:795:LYS:O	1:B:797:PHE:CE2	2.34	0.80
1:C:1031:GLU:O	1:C:1035:GLY:O	1.98	0.80
1:A:1022:ALA:HA	1:A:1025:ALA:CB	2.05	0.80
1:B:1082:CYS:SG	1:B:1126:CYS:HB2	2.20	0.80
1:C:781:VAL:CG2	1:C:1026:ALA:HB2	2.08	0.80
1:C:984:LEU:HG	1:C:988:GLU:HG2	1.64	0.80
1:A:726:ILE:HG23	1:A:948:LEU:CD1	2.11	0.80
1:B:353:TRP:CE3	1:B:466:ARG:HD3	2.16	0.80
1:C:429:PHE:CE1	1:C:431:GLY:O	2.34	0.80
1:B:126:VAL:HG22	1:B:172:SER:CB	2.11	0.80
1:B:342:PHE:CE2	1:B:368:LEU:HD12	2.16	0.80
1:B:1039:ARG:NH2	1:B:1042:PHE:CE2	2.49	0.80
1:A:308:VAL:HG22	1:A:602:THR:HB	1.63	0.80
1:A:453:TYR:CZ	1:A:493:GLN:HG3	2.17	0.80
1:B:365:TYR:CG	1:B:387:LEU:HB2	2.16	0.80
1:B:546:LEU:HD11	1:B:573:THR:OG1	1.82	0.80
1:C:37:TYR:HE1	1:C:55:PHE:CD1	1.99	0.80
1:A:332:ILE:H	1:A:332:ILE:HD12	1.46	0.80
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.16	0.80
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.16	0.80
1:B:539:VAL:HG12	1:B:550:GLY:O	1.81	0.80
1:B:599:THR:HG22	1:B:608:VAL:HG11	1.62	0.80
1:C:977:LEU:HD11	1:C:1000:ARG:NH1	1.95	0.80
1:A:299:THR:OG1	1:A:597:VAL:CG2	2.29	0.80
1:B:190:ARG:HE	1:B:207:HIS:CE1	1.98	0.80
1:C:220:PHE:CZ	1:C:288:ALA:HB3	2.17	0.80
1:A:317:ASN:CG	1:A:592:PHE:HZ	1.90	0.79
1:A:617:CYS:SG	1:A:644:GLN:HA	2.21	0.79
1:B:540:ASN:OD1	1:B:549:THR:HG23	1.82	0.79
1:B:615:VAL:CG1	1:B:620:VAL:CG1	2.57	0.79
1:B:1141:LEU:C	1:B:1145:LEU:HD23	2.06	0.79
1:C:374:PHE:CD2	1:C:436:TRP:CD1	2.70	0.79
1:B:289:VAL:HG23	1:B:306:PHE:CE2	2.17	0.79
1:C:83:VAL:HG21	1:C:237:ARG:NE	1.96	0.79
1:C:718:PHE:HZ	1:C:923:ILE:HG12	1.47	0.79
1:C:735:SER:HB3	1:C:861:LEU:CD2	2.10	0.79
1:A:435:ALA:CB	1:A:510:VAL:HG22	2.13	0.79
1:A:559:PHE:CD1	1:A:584:ILE:HD12	2.16	0.79
1:C:611:LEU:HB2	1:C:650:LEU:HD13	1.64	0.79
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.08	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG13	1:B:175:PHE:HE1	1.48	0.79
1:B:1140:PRO:C	1:B:1143:PRO:HD2	2.06	0.79
1:C:203:ILE:CG2	1:C:227:VAL:HG22	2.11	0.79
1:C:725:GLU:CD	1:C:1028:LYS:NZ	2.41	0.79
1:C:1089:PHE:O	1:C:1120:THR:CB	2.30	0.79
1:C:555:SER:OG	1:C:584:ILE:HG22	1.81	0.79
1:C:718:PHE:HZ	1:C:923:ILE:CG1	1.95	0.79
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.63	0.79
1:B:540:ASN:CG	1:B:549:THR:HG1	1.90	0.79
1:B:823:PHE:CZ	1:B:867:ASP:OD2	2.35	0.79
1:B:543:PHE:CG	1:B:576:VAL:CG2	2.65	0.79
1:C:612:TYR:CB	1:C:615:VAL:CG1	2.61	0.79
1:B:821:LEU:O	1:B:824:ASN:HB3	1.83	0.79
1:C:429:PHE:CE1	1:C:431:GLY:C	2.60	0.79
1:B:597:VAL:HG22	1:B:610:VAL:HG12	1.64	0.79
1:A:639:GLY:CA	1:A:642:VAL:HG23	2.14	0.79
1:B:329:PHE:CD2	1:B:330:PRO:CD	2.66	0.78
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.64	0.78
1:C:781:VAL:HG22	1:C:1026:ALA:CB	2.12	0.78
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.01	0.78
1:C:377:PHE:HD1	1:C:434:ILE:HG13	1.48	0.78
1:C:495:TYR:HD2	1:C:497:PHE:CE2	2.01	0.78
1:A:308:VAL:N	1:A:602:THR:HG21	1.99	0.78
1:C:552:LEU:CD2	1:C:587:ILE:CD1	2.62	0.78
1:C:105:ILE:HG13	1:C:118:LEU:HD11	1.66	0.78
1:C:350:VAL:CG1	1:C:422:ASN:CB	2.62	0.78
1:C:495:TYR:CD2	1:C:497:PHE:CE2	2.72	0.78
1:A:781:VAL:HA	1:A:1026:ALA:HA	1.64	0.78
1:A:1029:MET:SD	1:A:1060:VAL:CG1	2.69	0.78
1:C:36:VAL:O	1:C:223:LEU:HD23	1.83	0.78
1:A:353:TRP:HZ2	1:A:465:GLU:O	1.66	0.78
1:A:973:ILE:HG22	1:A:983:ARG:HH21	1.44	0.78
1:B:119:ILE:CD1	1:B:128:ILE:HG12	2.14	0.78
1:B:365:TYR:CD2	1:B:387:LEU:HB2	2.18	0.78
1:B:1095:PHE:HZ	1:B:1120:THR:HG21	1.46	0.78
1:C:105:ILE:HG21	1:C:135:PHE:CE2	2.17	0.78
1:C:612:TYR:CB	1:C:615:VAL:HG13	2.14	0.78
1:C:718:PHE:CZ	1:C:923:ILE:HG12	2.18	0.78
1:B:546:LEU:HD11	1:B:573:THR:CB	2.13	0.78
1:C:32:PHE:HB3	1:C:59:PHE:CD1	2.19	0.78
1:C:210:ILE:HD13	1:C:210:ILE:H	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.64	0.77
1:C:231:ILE:H	1:C:231:ILE:HD12	1.49	0.77
1:C:119:ILE:HD11	1:C:128:ILE:CA	2.12	0.77
1:C:552:LEU:HD22	1:C:587:ILE:HD11	1.66	0.77
1:A:552:LEU:CD2	1:A:587:ILE:HD13	2.06	0.77
1:A:743:CYS:SG	1:A:749:CYS:O	2.42	0.77
1:C:118:LEU:HD22	1:C:135:PHE:CE2	2.19	0.77
1:C:725:GLU:CD	1:C:1028:LYS:HZ1	1.92	0.77
1:A:83:VAL:CG2	1:A:237:ARG:HD3	2.09	0.77
1:C:965:GLN:HG3	1:C:970:PHE:HZ	1.50	0.77
1:B:1090:PRO:CD	1:B:1095:PHE:HE1	1.98	0.77
1:C:615:VAL:HG21	1:C:649:CYS:CB	2.06	0.77
1:C:736:VAL:HG21	1:C:858:LEU:HD12	1.67	0.77
1:C:87:ASN:CG	1:C:269:TYR:CE2	2.55	0.77
1:A:829:ALA:CB	1:A:949:GLN:OE1	2.32	0.77
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.67	0.77
1:C:921:LYS:HA	1:C:921:LYS:CE	2.15	0.77
1:B:743:CYS:SG	1:B:749:CYS:C	2.67	0.77
1:B:799:GLY:O	1:B:924:ALA:HB1	1.84	0.77
1:C:34:ARG:NH2	1:C:217:PRO:O	2.17	0.77
1:C:727:LEU:CD1	1:C:1028:LYS:HZ2	1.97	0.77
1:C:1103:PHE:HE1	1:C:1114:ILE:CD1	1.98	0.77
1:A:592:PHE:CG	1:A:593:GLY:N	2.46	0.77
1:C:654:GLU:OE1	1:C:654:GLU:N	2.18	0.76
1:C:931:ILE:O	1:C:934:ILE:HG23	1.84	0.76
1:C:984:LEU:HG	1:C:988:GLU:CG	2.15	0.76
1:C:1089:PHE:C	1:C:1120:THR:HB	2.10	0.76
1:A:976:VAL:HG13	1:A:979:ASP:CB	2.16	0.76
1:B:44:ARG:NH1	1:B:49:HIS:CD2	2.52	0.76
1:A:90:VAL:HG13	1:A:194:PHE:HB2	1.64	0.76
1:A:1088:HIS:CE1	1:A:1122:VAL:CG1	2.67	0.76
1:B:718:PHE:CZ	1:B:923:ILE:HD11	2.20	0.76
1:B:854:LYS:CB	1:B:858:LEU:O	2.34	0.76
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.66	0.76
1:A:34:ARG:HH12	1:A:217:PRO:HG2	1.48	0.76
1:C:977:LEU:CG	1:C:1000:ARG:HH12	1.96	0.76
1:A:1078:ALA:N	1:A:1102:TRP:HH2	1.83	0.76
1:A:727:LEU:C	1:A:948:LEU:HD21	2.11	0.76
1:B:426:PRO:CG	1:B:464:PHE:CD1	2.69	0.76
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.20	0.76
1:A:68:ILE:HA	1:A:261:GLY:O	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:O	1:A:949:GLN:N	2.17	0.76
1:A:1096:VAL:CG2	1:A:1105:THR:HG22	2.16	0.76
1:B:106:PHE:HZ	1:B:194:PHE:CD2	2.03	0.76
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.51	0.76
1:B:472:ILE:CG2	1:B:489:TYR:O	2.34	0.76
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.11	0.76
1:B:200:TYR:HE1	1:B:202:LYS:HG2	1.51	0.76
1:A:106:PHE:HZ	1:A:194:PHE:CD2	2.04	0.76
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.67	0.76
1:B:546:LEU:HD21	1:B:573:THR:HB	1.67	0.76
1:C:220:PHE:HE2	1:C:288:ALA:H	1.32	0.76
1:A:33:THR:HB	1:A:58:PHE:CE2	2.21	0.75
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.69	0.75
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.49	0.75
1:C:203:ILE:CG2	1:C:227:VAL:CG2	2.63	0.75
1:C:353:TRP:NE1	1:C:466:ARG:HB3	2.01	0.75
1:C:472:ILE:CG2	1:C:490:PHE:HA	2.15	0.75
1:A:91:TYR:CD1	1:A:193:VAL:HG22	2.21	0.75
1:C:89:GLY:C	1:C:270:LEU:CD1	2.58	0.75
1:C:541:PHE:HE2	1:C:587:ILE:CG2	1.99	0.75
1:C:905:ARG:CD	1:C:1049:LEU:O	2.34	0.75
1:C:1090:PRO:HB2	1:C:1093:GLY:O	1.86	0.75
1:C:736:VAL:HG23	1:C:857:GLY:O	1.85	0.75
1:A:327:VAL:HG23	1:A:529:LYS:O	1.86	0.75
1:A:331:ASN:CB	1:A:580:GLN:NE2	2.50	0.75
1:A:797:PHE:HE1	1:A:882:ILE:CG2	1.97	0.75
1:C:324:GLU:O	1:C:539:VAL:HB	1.86	0.75
1:A:119:ILE:CG1	1:A:128:ILE:HG12	2.16	0.75
1:A:331:ASN:CG	1:A:580:GLN:HE21	1.95	0.75
1:B:726:ILE:HG21	1:B:948:LEU:HD12	1.68	0.75
1:A:403:ARG:HG3	1:A:495:TYR:OH	1.87	0.75
1:B:521:PRO:HB3	1:B:544:ASN:ND2	2.00	0.75
1:C:204:TYR:CD1	1:C:225:PRO:HB3	2.21	0.75
1:C:773:GLU:OE2	1:C:1019:ARG:CD	2.34	0.75
1:A:108:THR:OG1	1:A:234:ASN:O	2.04	0.74
1:B:1089:PHE:O	1:B:1120:THR:HB	1.87	0.74
1:C:83:VAL:CG2	1:C:237:ARG:NH2	2.50	0.74
1:A:88:ASP:OD1	1:A:88:ASP:N	2.20	0.74
1:A:559:PHE:HD1	1:A:584:ILE:HD12	1.51	0.74
1:C:33:THR:CB	1:C:58:PHE:CE1	2.68	0.74
1:B:1029:MET:HE2	1:B:1062:PHE:CZ	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:CB	1:A:275:PHE:CE2	2.69	0.74
1:A:885:GLY:HA2	1:A:901:GLN:HE22	1.48	0.74
1:C:32:PHE:HE1	1:C:218:GLN:HB3	1.52	0.74
1:C:763:LEU:HD22	1:C:1008:VAL:CG2	2.15	0.74
1:A:96:GLU:C	1:A:186:PHE:HD2	1.95	0.74
1:B:370:ASN:O	1:B:372:ALA:N	2.19	0.74
1:B:501:ASN:HB3	1:B:505:TYR:HB3	1.70	0.74
1:A:453:TYR:CZ	1:A:493:GLN:CG	2.71	0.74
1:B:543:PHE:CE2	1:B:585:LEU:HD12	2.22	0.74
1:C:490:PHE:CE1	1:C:491:PRO:HD2	2.20	0.74
1:A:231:ILE:HG22	1:A:233:ILE:H	1.51	0.74
1:A:326:ILE:HG21	1:A:534:VAL:HG22	1.68	0.74
1:B:152:TRP:HH2	1:B:245:HIS:CE1	2.06	0.74
1:A:55:PHE:CG	1:A:275:PHE:CE2	2.76	0.74
1:B:541:PHE:CE2	1:B:587:ILE:HG23	2.22	0.74
1:C:37:TYR:CD1	1:C:55:PHE:CE1	2.69	0.74
1:C:727:LEU:HD11	1:C:1028:LYS:CE	2.17	0.74
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.70	0.74
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.22	0.74
1:A:90:VAL:HG11	1:A:194:PHE:HB2	1.69	0.73
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.70	0.73
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.69	0.73
1:C:612:TYR:HB3	1:C:615:VAL:HG13	1.70	0.73
1:B:472:ILE:HG23	1:B:489:TYR:C	2.12	0.73
1:A:1048:HIS:ND1	1:A:1048:HIS:O	2.20	0.73
1:C:858:LEU:HD23	1:C:959:LEU:HD11	1.71	0.73
1:B:985:ASP:C	1:B:989:ALA:HB2	2.11	0.73
1:C:119:ILE:CD1	1:C:128:ILE:CB	2.67	0.73
1:C:715:PRO:HA	1:C:1071:GLN:O	1.87	0.73
1:C:763:LEU:HD13	1:C:1004:LEU:HD21	1.69	0.73
1:B:351:TYR:HB3	1:B:422:ASN:ND2	2.03	0.73
1:B:1080:ALA:HB2	1:B:1089:PHE:HE1	1.53	0.73
1:C:605:SER:OG	1:C:607:GLN:HG2	1.88	0.73
1:B:107:GLY:O	1:B:235:ILE:HG23	1.87	0.73
1:B:722:VAL:HG23	1:B:930:ALA:HB1	1.69	0.73
1:C:472:ILE:HG22	1:C:490:PHE:HD1	1.54	0.73
1:C:1080:ALA:O	1:C:1132:ILE:HG13	1.89	0.73
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.71	0.73
1:C:902:MET:CB	1:C:916:LEU:HD21	2.11	0.73
1:B:817:PHE:CZ	1:B:935:GLN:NE2	2.57	0.73
1:B:1141:LEU:HG	1:B:1145:LEU:HD21	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:H	1:C:523:THR:HG23	1.54	0.73
1:C:555:SER:OG	1:C:584:ILE:C	2.32	0.73
1:A:90:VAL:CG1	1:A:194:PHE:O	2.37	0.73
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.23	0.73
1:B:902:MET:HB3	1:B:916:LEU:CD2	2.19	0.73
1:B:1029:MET:HE1	1:B:1053:PRO:HB3	1.68	0.73
1:C:33:THR:H	1:C:58:PHE:HD1	1.36	0.73
1:C:989:ALA:O	1:C:993:ILE:CB	2.37	0.73
1:A:328:ARG:HH22	1:A:533:LEU:CB	2.02	0.73
1:C:328:ARG:HB3	1:C:578:ASP:OD1	1.88	0.73
1:C:612:TYR:HB2	1:C:615:VAL:HG11	1.69	0.73
1:A:829:ALA:HB3	1:A:949:GLN:OE1	1.89	0.72
1:B:126:VAL:CG2	1:B:172:SER:HB3	2.16	0.72
1:C:69:HIS:HA	1:C:78:ARG:O	1.88	0.72
1:C:644:GLN:NE2	1:C:644:GLN:HA	2.02	0.72
1:C:989:ALA:O	1:C:993:ILE:HB	1.89	0.72
1:A:1088:HIS:CE1	1:A:1122:VAL:HG11	2.24	0.72
1:C:462:LYS:HA	1:C:462:LYS:CE	2.16	0.72
1:C:712:ILE:CD1	1:C:1094:VAL:HG11	2.18	0.72
1:A:620:VAL:CG2	1:A:621:PRO:CD	2.68	0.72
1:B:316:SER:O	1:B:595:VAL:HG22	1.89	0.72
1:B:318:PHE:HE2	1:B:615:VAL:HG21	1.54	0.72
1:B:426:PRO:HG2	1:B:464:PHE:CE2	2.21	0.72
1:B:743:CYS:SG	1:B:750:SER:CA	2.78	0.72
1:C:326:ILE:HD11	1:C:552:LEU:CD1	2.19	0.72
1:A:331:ASN:N	1:A:580:GLN:NE2	2.37	0.72
1:B:195:LYS:CD	1:B:197:ILE:HD11	2.19	0.72
1:B:317:ASN:ND2	1:C:737:ASP:CG	2.45	0.72
1:B:324:GLU:O	1:B:539:VAL:HG23	1.88	0.72
1:B:805:ILE:HA	1:B:818:ILE:CD1	2.19	0.72
1:A:321:GLN:HA	1:A:321:GLN:HE21	1.53	0.72
1:B:539:VAL:O	1:B:550:GLY:N	2.22	0.72
1:C:1083:HIS:HB2	1:C:1137:VAL:CG2	2.19	0.72
1:B:386:LYS:CE	1:C:982:SER:O	2.37	0.72
1:B:746:SER:O	1:B:749:CYS:SG	2.47	0.72
1:A:1090:PRO:HB2	1:A:1093:GLY:O	1.89	0.72
1:A:1138:TYR:HE2	1:A:1140:PRO:HB3	1.55	0.72
1:B:1088:HIS:ND1	1:B:1122:VAL:HG23	2.04	0.72
1:C:611:LEU:HB2	1:C:650:LEU:CD1	2.19	0.72
1:B:540:ASN:CG	1:B:549:THR:OG1	2.33	0.72
1:B:730:SER:O	1:B:1058:HIS:HB3	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:CYS:SG	1:B:760:CYS:O	2.48	0.72
1:C:33:THR:CG2	1:C:58:PHE:CE1	2.73	0.72
1:C:105:ILE:CG2	1:C:135:PHE:HE2	2.03	0.72
1:C:203:ILE:HG22	1:C:227:VAL:HG23	1.70	0.72
1:A:403:ARG:CG	1:A:495:TYR:CE1	2.73	0.71
1:B:351:TYR:HB3	1:B:422:ASN:HD22	1.54	0.71
1:C:541:PHE:CD2	1:C:552:LEU:CD2	2.61	0.71
1:C:327:VAL:CG1	1:C:329:PHE:CE2	2.72	0.71
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.55	0.71
1:B:322:PRO:HB3	1:B:549:THR:CG2	2.21	0.71
1:B:815:ARG:NH1	1:B:823:PHE:CG	2.59	0.71
1:C:90:VAL:N	1:C:270:LEU:HD13	2.05	0.71
1:C:897:PRO:HG2	1:C:900:MET:SD	2.30	0.71
1:C:912:THR:HG23	1:C:1106:GLN:OE1	1.91	0.71
1:B:617:CYS:SG	1:B:644:GLN:HG2	2.30	0.71
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.55	0.71
1:C:615:VAL:CG2	1:C:649:CYS:HB2	2.12	0.71
1:B:197:ILE:HB	1:B:202:LYS:CE	2.15	0.71
1:C:411:ALA:C	1:C:425:LEU:HD12	2.15	0.71
1:A:736:VAL:CG2	1:A:858:LEU:HD22	2.19	0.71
1:A:784:GLN:NE2	1:A:1030:SER:HB2	2.06	0.71
1:A:970:PHE:HE1	1:B:756:TYR:O	1.73	0.71
1:B:577:ARG:HB2	1:B:584:ILE:HG13	1.70	0.71
1:B:616:ASN:C	1:B:649:CYS:SG	2.73	0.71
1:A:724:THR:HG22	1:A:1063:LEU:CD2	2.19	0.71
1:B:200:TYR:CE1	1:B:202:LYS:HE2	2.25	0.71
1:B:396:TYR:CE2	1:C:200:TYR:OH	2.43	0.71
1:B:800:PHE:CD2	1:B:927:PHE:CD2	2.79	0.71
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.23	0.71
1:B:1090:PRO:HD3	1:B:1095:PHE:CE1	2.24	0.71
1:C:599:THR:HB	1:C:608:VAL:HG12	1.72	0.71
1:C:726:ILE:HG22	1:C:948:LEU:HG	1.71	0.71
1:C:878:LEU:HD23	1:C:1053:PRO:HD2	1.71	0.71
1:C:1090:PRO:HA	1:C:1120:THR:CG2	2.07	0.71
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.21	0.71
1:A:985:ASP:OD1	1:A:986:PRO:CD	2.38	0.71
1:B:365:TYR:CD1	1:B:387:LEU:HD13	2.26	0.71
1:C:101:ILE:HD11	1:C:263:ALA:HB1	1.73	0.71
1:A:86:PHE:HE2	1:A:90:VAL:HG11	1.55	0.71
1:A:959:LEU:O	1:A:963:VAL:HG23	1.91	0.71
1:B:89:GLY:C	1:B:270:LEU:HD13	2.16	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:GLY:CA	1:A:901:GLN:NE2	2.43	0.71
1:C:55:PHE:CB	1:C:275:PHE:CE1	2.73	0.71
1:C:203:ILE:HG22	1:C:227:VAL:CG2	2.21	0.71
1:C:607:GLN:NE2	1:C:674:TYR:CZ	2.57	0.71
1:C:773:GLU:OE2	1:C:1019:ARG:CG	2.39	0.71
1:A:64:TRP:NE1	1:A:266:TYR:CZ	2.59	0.70
1:A:92:PHE:CE1	1:A:94:SER:HB3	2.26	0.70
1:A:118:LEU:HD22	1:A:135:PHE:CE1	2.25	0.70
1:A:1043:CYS:C	1:A:1064:HIS:HD1	1.99	0.70
1:A:1091:ARG:CZ	1:A:1118:ASP:O	2.39	0.70
1:B:324:GLU:O	1:B:539:VAL:HG22	1.89	0.70
1:B:662:CYS:CB	1:B:671:CYS:HG	2.04	0.70
1:B:722:VAL:HG12	1:B:934:ILE:HG13	1.71	0.70
1:B:1028:LYS:NZ	1:B:1042:PHE:HD1	1.86	0.70
1:C:878:LEU:CD2	1:C:1053:PRO:HD2	2.21	0.70
1:A:308:VAL:C	1:A:602:THR:HG22	2.16	0.70
1:A:742:ILE:HD13	1:A:1001:LEU:HD23	1.72	0.70
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.26	0.70
1:C:541:PHE:CE2	1:C:552:LEU:CD2	2.70	0.70
1:C:736:VAL:HG21	1:C:858:LEU:CD1	2.21	0.70
1:A:826:VAL:CG2	1:A:945:LEU:CD1	2.68	0.70
1:B:823:PHE:HA	1:B:826:VAL:HG12	1.71	0.70
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.73	0.70
1:B:993:ILE:O	1:B:997:ILE:HG12	1.91	0.70
1:B:105:ILE:HG13	1:B:118:LEU:HD13	1.72	0.70
1:C:495:TYR:CD2	1:C:497:PHE:HE2	2.06	0.70
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.24	0.70
1:A:826:VAL:HG23	1:A:945:LEU:CD1	2.20	0.70
1:B:92:PHE:CZ	1:B:265:TYR:CD2	2.74	0.70
1:B:905:ARG:HD2	1:B:1049:LEU:O	1.92	0.70
1:B:1088:HIS:CE1	1:B:1122:VAL:CG2	2.74	0.70
1:C:87:ASN:OD1	1:C:87:ASN:N	2.25	0.70
1:C:282:ASN:OD1	1:C:282:ASN:N	2.23	0.70
1:A:1081:ILE:CG2	1:A:1135:ASN:HB3	2.21	0.70
1:B:53:ASP:O	1:B:55:PHE:CD2	2.45	0.70
1:B:1105:THR:HB	1:B:1111:GLU:O	1.92	0.70
1:C:289:VAL:CG2	1:C:306:PHE:CZ	2.67	0.70
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.73	0.70
1:B:726:ILE:HG21	1:B:948:LEU:CG	2.22	0.70
1:B:821:LEU:CD1	1:B:824:ASN:HD22	2.05	0.70
1:C:204:TYR:CE1	1:C:225:PRO:HB3	2.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.74	0.70
1:A:90:VAL:CG2	1:A:238:PHE:CE2	2.74	0.70
1:A:133:PHE:CE1	1:A:163:ALA:HB2	2.26	0.70
1:B:329:PHE:C	1:B:579:PRO:CG	2.61	0.70
1:B:821:LEU:CD1	1:B:824:ASN:ND2	2.54	0.70
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.74	0.70
1:A:93:ALA:O	1:A:266:TYR:HD1	1.75	0.69
1:C:100:ILE:HA	1:C:243:ALA:HB3	1.74	0.69
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.27	0.69
1:A:781:VAL:CG1	1:A:1029:MET:CG	2.69	0.69
1:A:1028:LYS:C	1:A:1062:PHE:CE2	2.71	0.69
1:C:294:ASP:OD1	1:C:297:SER:OG	2.08	0.69
1:C:86:PHE:CD2	1:C:90:VAL:HG21	2.27	0.69
1:C:426:PRO:HG2	1:C:464:PHE:CD2	2.27	0.69
1:C:503:VAL:HA	1:C:506:GLN:OE1	1.92	0.69
1:C:643:PHE:CE1	1:C:655:HIS:CG	2.80	0.69
1:C:654:GLU:OE1	1:C:692:ILE:O	2.09	0.69
1:A:203:ILE:HG22	1:A:227:VAL:HG23	1.73	0.69
1:B:957:GLN:O	1:B:961:THR:OG1	2.09	0.69
1:C:46:SER:HA	1:C:279:TYR:O	1.92	0.69
1:A:529:LYS:O	1:A:530:SER:C	2.30	0.69
1:B:515:PHE:C	1:B:516:GLU:CD	2.59	0.69
1:B:654:GLU:O	1:B:693:ILE:HA	1.93	0.69
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.72	0.69
1:B:819:GLU:CG	1:B:1054:GLN:OE1	2.39	0.69
1:A:68:ILE:HB	1:A:262:ALA:HA	1.74	0.69
1:C:1103:PHE:HE1	1:C:1114:ILE:HD13	1.58	0.69
1:A:220:PHE:HZ	1:A:288:ALA:HB3	1.56	0.69
1:A:329:PHE:CE2	1:A:528:LYS:HG3	2.26	0.69
1:A:551:VAL:C	1:A:552:LEU:HD23	2.18	0.69
1:B:543:PHE:HB3	1:B:576:VAL:HG21	0.88	0.69
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.11	0.69
1:B:1028:LYS:HD2	1:B:1032:CYS:SG	2.29	0.69
1:C:956:ALA:O	1:C:960:ASN:CB	2.41	0.69
1:A:773:GLU:OE2	1:A:1019:ARG:HB2	1.93	0.69
1:A:1138:TYR:CE2	1:A:1140:PRO:HA	2.26	0.69
1:B:322:PRO:CG	1:B:549:THR:CG2	2.62	0.69
1:B:470:THR:HG22	1:B:492:LEU:HD12	1.73	0.69
1:C:360:ASN:HA	1:C:523:THR:HG21	1.75	0.69
1:C:551:VAL:HG13	1:C:590:CYS:SG	2.32	0.69
1:C:588:THR:HG22	1:C:589:PRO:HD2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD12	1:A:262:ALA:HB2	1.74	0.69
1:A:1033:VAL:HG12	1:A:1034:LEU:HD23	1.75	0.69
1:A:1089:PHE:HB2	1:A:1121:PHE:HE1	1.58	0.69
1:B:718:PHE:HD2	1:B:1067:TYR:CD1	2.10	0.69
1:C:551:VAL:O	1:C:587:ILE:HA	1.92	0.69
1:C:1140:PRO:O	1:C:1143:PRO:HD2	1.93	0.69
1:A:1138:TYR:CE2	1:A:1140:PRO:HB3	2.27	0.69
1:B:55:PHE:CB	1:B:275:PHE:HE2	2.06	0.69
1:B:106:PHE:CB	1:B:235:ILE:HD13	2.20	0.69
1:B:658:ASN:OD1	1:B:658:ASN:N	2.25	0.69
1:B:1011:GLN:HA	1:B:1011:GLN:NE2	2.06	0.69
1:C:48:LEU:HD12	1:C:48:LEU:H	1.57	0.69
1:C:336:CYS:SG	1:C:361:CYS:C	2.76	0.69
1:C:458:LYS:CA	1:C:473:TYR:HE1	2.06	0.69
1:C:340:GLU:OE2	1:C:356:LYS:NZ	2.26	0.68
1:C:380:TYR:HE2	1:C:412:PRO:CD	2.04	0.68
1:C:541:PHE:CZ	1:C:587:ILE:HG21	2.27	0.68
1:C:736:VAL:CG2	1:C:858:LEU:CD1	2.71	0.68
1:B:1031:GLU:OE2	1:B:1039:ARG:HD3	1.92	0.68
1:C:119:ILE:HG12	1:C:128:ILE:CA	2.22	0.68
1:C:220:PHE:HE2	1:C:287:ASP:OD1	1.75	0.68
1:C:973:ILE:HG13	1:C:980:ILE:HD12	1.73	0.68
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.74	0.68
1:A:895:GLN:OE1	1:A:895:GLN:N	2.24	0.68
1:B:89:GLY:O	1:B:270:LEU:HD12	1.94	0.68
1:B:89:GLY:O	1:B:270:LEU:CD1	2.41	0.68
1:C:119:ILE:CD1	1:C:128:ILE:HG12	2.22	0.68
1:C:643:PHE:CZ	1:C:655:HIS:CG	2.82	0.68
1:C:726:ILE:CG2	1:C:948:LEU:HG	2.22	0.68
1:C:989:ALA:O	1:C:993:ILE:HG12	1.93	0.68
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.27	0.68
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.27	0.68
1:A:826:VAL:CG1	1:A:1057:PRO:HG2	2.24	0.68
1:B:298:GLU:CD	1:B:315:THR:HG21	2.17	0.68
1:A:781:VAL:HG13	1:A:1029:MET:HG3	1.75	0.68
1:A:1096:VAL:HG21	1:A:1105:THR:CG2	2.22	0.68
1:B:722:VAL:HG23	1:B:930:ALA:CB	2.24	0.68
1:B:1142:GLN:HA	1:B:1142:GLN:HE21	1.56	0.68
1:C:273:ARG:NH1	1:C:292:ALA:CB	2.56	0.68
1:C:905:ARG:HE	1:C:1050:MET:HE2	1.57	0.68
1:A:90:VAL:HG12	1:A:194:PHE:O	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.24	0.68
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.73	0.68
1:A:673:SER:O	1:A:693:ILE:CD1	2.42	0.68
1:C:390:LEU:HD12	1:C:390:LEU:O	1.93	0.68
1:C:977:LEU:HG	1:C:1000:ARG:NH2	2.07	0.68
1:A:726:ILE:HG23	1:A:948:LEU:HD11	1.76	0.68
1:A:782:PHE:CZ	1:A:1060:VAL:HG22	2.28	0.68
1:B:815:ARG:CZ	1:B:823:PHE:CD2	2.76	0.68
1:B:818:ILE:HD12	1:B:1054:GLN:NE2	2.08	0.68
1:C:392:PHE:CD2	1:C:395:VAL:CG2	2.70	0.68
1:A:55:PHE:CG	1:A:275:PHE:CD2	2.81	0.68
1:B:718:PHE:HZ	1:B:923:ILE:CD1	2.05	0.68
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.59	0.68
1:A:675:GLN:HA	1:A:675:GLN:HE21	1.58	0.68
1:B:126:VAL:HG13	1:B:175:PHE:CZ	2.29	0.68
1:C:203:ILE:HG21	1:C:227:VAL:HG22	1.74	0.68
1:C:348:ALA:O	1:C:400:PHE:HA	1.93	0.68
1:C:748:GLU:HG3	1:C:981:LEU:HD21	1.76	0.68
1:C:318:PHE:CE1	1:C:593:GLY:HA3	2.29	0.68
1:C:643:PHE:HZ	1:C:655:HIS:ND1	1.92	0.68
1:C:921:LYS:HA	1:C:921:LYS:HE2	1.76	0.68
1:C:1030:SER:O	1:C:1034:LEU:HB2	1.94	0.68
1:B:44:ARG:HB3	1:B:47:VAL:HG21	1.75	0.67
1:B:275:PHE:HD1	1:B:290:ASP:HA	1.59	0.67
1:B:393:THR:CG2	1:B:522:ALA:HB2	2.21	0.67
1:C:347:PHE:CZ	1:C:509:ARG:HD3	2.29	0.67
1:C:471:GLU:O	1:C:491:PRO:CB	2.42	0.67
1:A:331:ASN:CB	1:A:580:GLN:HE21	2.06	0.67
1:A:521:PRO:CG	1:A:564:GLN:HG3	2.23	0.67
1:A:597:VAL:HG12	1:A:610:VAL:HG22	1.77	0.67
1:A:992:GLN:HA	1:A:992:GLN:NE2	2.09	0.67
1:B:386:LYS:HE3	1:C:982:SER:O	1.94	0.67
1:B:131:CYS:HG	1:B:166:CYS:HG	1.39	0.67
1:B:365:TYR:CE2	1:B:387:LEU:C	2.72	0.67
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.77	0.67
1:A:394:ASN:HD21	1:B:230:PRO:CB	2.07	0.67
1:B:126:VAL:HG23	1:B:172:SER:HB2	1.75	0.67
1:C:734:THR:HG23	1:C:767:LEU:CD1	2.24	0.67
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.58	0.67
1:B:50:SER:HA	1:B:275:PHE:O	1.94	0.67
1:B:1141:LEU:C	1:B:1145:LEU:CD2	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HB3	1:C:289:VAL:HB	1.77	0.67
1:A:327:VAL:HB	1:A:329:PHE:CE2	2.30	0.67
1:B:564:GLN:HE21	1:B:564:GLN:HA	1.59	0.67
1:B:615:VAL:O	1:B:649:CYS:SG	2.52	0.67
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	1.77	0.67
1:C:119:ILE:HD11	1:C:128:ILE:HA	1.71	0.67
1:C:457:ARG:C	1:C:473:TYR:CE1	2.73	0.67
1:A:90:VAL:HG23	1:A:238:PHE:HE2	1.56	0.67
1:B:501:ASN:HB3	1:B:505:TYR:CB	2.25	0.67
1:B:534:VAL:O	1:B:552:LEU:HB2	1.94	0.67
1:B:816:SER:OG	1:B:819:GLU:HG3	1.95	0.67
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.30	0.67
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.77	0.67
1:A:97:LYS:HD3	1:A:98:SER:OG	1.95	0.67
1:A:735:SER:HB2	1:A:859:THR:HG23	1.76	0.67
1:A:896:ILE:HG22	1:A:897:PRO:HD2	1.77	0.67
1:C:294:ASP:OD1	1:C:297:SER:N	2.23	0.67
1:A:829:ALA:C	1:A:949:GLN:OE1	2.38	0.66
1:B:728:PRO:HD2	1:B:1021:SER:OG	1.93	0.66
1:B:856:ASN:OD1	1:B:857:GLY:N	2.28	0.66
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.28	0.66
1:C:959:LEU:O	1:C:963:VAL:HG23	1.95	0.66
1:B:69:HIS:CE1	1:B:77:LYS:H	2.14	0.66
1:B:118:LEU:HB2	1:B:135:PHE:HZ	1.60	0.66
1:B:331:ASN:C	1:B:333:THR:HG23	2.20	0.66
1:B:584:ILE:H	1:B:584:ILE:HD12	1.61	0.66
1:C:327:VAL:HG11	1:C:329:PHE:CE2	2.30	0.66
1:C:692:ILE:HD12	1:C:692:ILE:H	1.61	0.66
1:A:166:CYS:HB2	1:A:169:GLU:OE2	1.95	0.66
1:A:1095:PHE:HB3	1:A:1102:TRP:CZ3	2.30	0.66
1:B:164:ASN:OD1	1:B:165:ASN:CG	2.39	0.66
1:B:914:ASN:OD1	1:B:915:VAL:N	2.28	0.66
1:C:1092:GLU:OE2	1:C:1106:GLN:HB3	1.95	0.66
1:A:308:VAL:H	1:A:602:THR:HG21	1.58	0.66
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.28	0.66
1:B:322:PRO:HB3	1:B:549:THR:HG23	1.76	0.66
1:B:822:LEU:HD21	1:B:1056:ALA:CB	2.18	0.66
1:C:105:ILE:CB	1:C:118:LEU:HD13	2.25	0.66
1:C:119:ILE:CD1	1:C:128:ILE:CA	2.67	0.66
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.11	0.66
1:A:90:VAL:N	1:A:270:LEU:HD13	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:ARG:NH1	1:B:823:PHE:CE2	2.64	0.66
1:B:1105:THR:CB	1:B:1111:GLU:O	2.44	0.66
1:C:379:CYS:SG	1:C:382:VAL:O	2.53	0.66
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.59	0.66
1:A:617:CYS:SG	1:A:644:GLN:OE1	2.54	0.66
1:B:659:SER:CB	1:B:698:SER:HB3	2.25	0.66
1:B:1028:LYS:NZ	1:B:1042:PHE:C	2.53	0.66
1:C:220:PHE:HZ	1:C:288:ALA:HB3	1.51	0.66
1:C:334:ASN:N	1:C:334:ASN:OD1	2.29	0.66
1:C:458:LYS:N	1:C:473:TYR:CE1	2.62	0.66
1:C:541:PHE:CE2	1:C:587:ILE:CG2	2.75	0.66
1:B:365:TYR:CD1	1:B:387:LEU:CD1	2.79	0.66
1:B:856:ASN:C	1:B:858:LEU:N	2.49	0.66
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.78	0.66
1:A:988:GLU:O	1:A:991:VAL:HG13	1.96	0.66
1:A:308:VAL:H	1:A:602:THR:CG2	2.09	0.65
1:A:319:ARG:CG	1:A:592:PHE:CD2	2.75	0.65
1:C:387:LEU:HD23	1:C:390:LEU:HD11	1.78	0.65
1:C:729:VAL:O	1:C:1022:ALA:HB2	1.96	0.65
1:C:773:GLU:OE2	1:C:1019:ARG:HD2	1.95	0.65
1:B:69:HIS:HA	1:B:78:ARG:O	1.95	0.65
1:B:204:TYR:HD1	1:B:225:PRO:CA	2.08	0.65
1:B:317:ASN:ND2	1:C:737:ASP:HB2	2.11	0.65
1:B:909:ILE:HG23	1:B:1036:GLN:NE2	2.11	0.65
1:C:105:ILE:HD11	1:C:241:LEU:HD13	1.76	0.65
1:C:659:SER:CB	1:C:698:SER:HB3	2.26	0.65
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.30	0.65
1:B:335:LEU:C	1:B:361:CYS:HB2	2.20	0.65
1:B:543:PHE:HB2	1:B:576:VAL:CG2	1.96	0.65
1:A:89:GLY:HA2	1:A:270:LEU:CB	2.23	0.65
1:B:97:LYS:HD3	1:B:98:SER:OG	1.96	0.65
1:C:327:VAL:HG12	1:C:329:PHE:CE2	2.31	0.65
1:A:220:PHE:HE2	1:A:288:ALA:H	1.44	0.65
1:A:330:PRO:HA	1:A:580:GLN:OE1	1.97	0.65
1:C:395:VAL:HG21	1:C:524:VAL:HG11	1.78	0.65
1:B:543:PHE:CD1	1:B:576:VAL:CG1	2.71	0.65
1:B:743:CYS:O	1:B:749:CYS:SG	2.54	0.65
1:C:100:ILE:HD12	1:C:243:ALA:O	1.97	0.65
1:A:353:TRP:CZ2	1:A:465:GLU:C	2.73	0.65
1:A:729:VAL:CG2	1:A:1060:VAL:HG23	2.25	0.65
1:B:123:ALA:O	1:B:175:PHE:O	2.15	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.28	0.65
1:B:393:THR:HG23	1:B:522:ALA:CB	2.22	0.65
1:B:797:PHE:CB	1:B:800:PHE:O	2.45	0.65
1:B:985:ASP:C	1:B:987:PRO:HD2	2.21	0.65
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.77	0.65
1:B:204:TYR:CD1	1:B:225:PRO:CA	2.80	0.65
1:B:365:TYR:HE2	1:B:388:ASN:HA	1.61	0.65
1:B:502:GLY:O	1:B:505:TYR:N	2.30	0.65
1:B:708:SER:HB2	1:B:711:SER:OG	1.97	0.65
1:C:360:ASN:ND2	1:C:523:THR:HG21	2.09	0.65
1:C:296:LEU:HD13	1:C:608:VAL:HG11	1.79	0.65
1:C:360:ASN:H	1:C:523:THR:CG2	2.10	0.65
1:A:86:PHE:HB3	1:A:237:ARG:HA	1.78	0.64
1:A:235:ILE:H	1:A:235:ILE:HD12	1.62	0.64
1:B:119:ILE:CD1	1:B:128:ILE:HG23	2.17	0.64
1:C:126:VAL:HG13	1:C:175:PHE:CZ	2.32	0.64
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.32	0.64
1:A:89:GLY:C	1:A:270:LEU:HD12	2.22	0.64
1:A:220:PHE:CZ	1:A:288:ALA:HB3	2.32	0.64
1:A:308:VAL:N	1:A:602:THR:CG2	2.60	0.64
1:A:403:ARG:HD3	1:A:495:TYR:HE1	1.62	0.64
1:A:1030:SER:O	1:A:1034:LEU:HG	1.97	0.64
1:B:382:VAL:CG2	1:C:983:ARG:O	2.39	0.64
1:B:538:CYS:CA	1:B:551:VAL:HG12	2.26	0.64
1:B:816:SER:N	1:B:819:GLU:HB2	2.11	0.64
1:A:480:CYS:SG	1:A:488:CYS:HA	2.37	0.64
1:B:559:PHE:CD1	1:B:584:ILE:HG12	2.31	0.64
1:A:781:VAL:HG22	1:A:1026:ALA:N	2.12	0.64
1:B:738:CYS:SG	1:B:760:CYS:C	2.80	0.64
1:B:784:GLN:HA	1:B:784:GLN:NE2	2.08	0.64
1:B:985:ASP:OD1	1:B:987:PRO:HD2	1.96	0.64
1:C:69:HIS:CE1	1:C:77:LYS:H	2.14	0.64
1:C:590:CYS:HB3	1:C:619:GLU:OE2	1.97	0.64
1:C:660:TYR:O	1:C:695:TYR:HE2	1.80	0.64
1:A:92:PHE:CZ	1:A:94:SER:HB3	2.33	0.64
1:A:133:PHE:CZ	1:A:160:TYR:CE1	2.86	0.64
1:A:353:TRP:CD2	1:A:466:ARG:HD3	2.31	0.64
1:B:275:PHE:CE1	1:B:290:ASP:HA	2.32	0.64
1:B:360:ASN:OD1	1:B:523:THR:HG21	1.95	0.64
1:C:524:VAL:O	1:C:524:VAL:HG12	1.97	0.64
1:A:650:LEU:HD21	1:A:666:ILE:HD13	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:VAL:HG22	1:A:1022:ALA:O	1.98	0.64
1:A:782:PHE:CE2	1:A:870:ILE:HG23	2.33	0.64
1:B:543:PHE:HZ	1:B:585:LEU:HD12	1.60	0.64
1:C:43:PHE:HE1	1:C:45:SER:HB3	1.61	0.64
1:C:203:ILE:HG21	1:C:227:VAL:CG2	2.27	0.64
1:C:472:ILE:HG22	1:C:490:PHE:CD1	2.32	0.64
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.33	0.64
1:A:781:VAL:HG13	1:A:1029:MET:CG	2.26	0.64
1:C:273:ARG:HH11	1:C:292:ALA:HB3	1.60	0.64
1:A:1105:THR:CB	1:A:1111:GLU:O	2.46	0.64
1:C:34:ARG:O	1:C:56:LEU:HD23	1.98	0.64
1:C:584:ILE:C	1:C:585:LEU:HD23	2.23	0.64
1:C:989:ALA:O	1:C:993:ILE:N	2.26	0.64
1:A:474:GLN:OE1	1:A:479:PRO:HB3	1.98	0.64
1:A:521:PRO:HG3	1:A:564:GLN:CG	2.24	0.64
1:A:590:CYS:O	1:A:591:SER:O	2.14	0.64
1:A:970:PHE:CE1	1:B:756:TYR:O	2.50	0.64
1:A:1082:CYS:HB2	1:A:1132:ILE:CD1	2.28	0.64
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.28	0.64
1:B:1102:TRP:CB	1:B:1135:ASN:HD22	2.06	0.64
1:A:29:THR:O	1:A:62:VAL:CG1	2.47	0.64
1:A:280:ASN:ND2	1:A:286:THR:HG21	2.13	0.64
1:A:329:PHE:CZ	1:A:528:LYS:HG3	2.32	0.63
1:B:334:ASN:HB2	1:B:361:CYS:HA	1.81	0.63
1:B:546:LEU:HB3	1:B:565:PHE:CE1	2.32	0.63
1:B:1122:VAL:O	1:B:1122:VAL:HG22	1.99	0.63
1:C:55:PHE:HB2	1:C:275:PHE:CE1	2.33	0.63
1:C:730:SER:HB2	1:C:774:GLN:HB3	1.80	0.63
1:C:973:ILE:HG23	1:C:992:GLN:HE22	1.61	0.63
1:A:220:PHE:CE2	1:A:288:ALA:N	2.66	0.63
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.34	0.63
1:A:718:PHE:HD2	1:A:1109:PHE:HE2	1.44	0.63
1:B:638:THR:O	1:B:642:VAL:HG11	1.99	0.63
1:B:1114:ILE:CG2	1:B:1138:TYR:CD1	2.81	0.63
1:C:119:ILE:CG1	1:C:127:VAL:C	2.70	0.63
1:B:474:GLN:OE1	1:B:479:PRO:HB3	1.98	0.63
1:C:91:TYR:N	1:C:268:GLY:O	2.29	0.63
1:C:117:LEU:HD23	1:C:117:LEU:C	2.23	0.63
1:C:118:LEU:HD22	1:C:135:PHE:CE1	2.31	0.63
1:A:763:LEU:HD13	1:A:1004:LEU:HD13	1.80	0.63
1:A:823:PHE:O	1:A:827:THR:HG23	1.94	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:LEU:HD12	1:A:962:LEU:O	1.99	0.63
1:B:212:LEU:HD13	1:B:212:LEU:C	2.23	0.63
1:B:612:TYR:O	1:B:648:GLY:HA3	1.98	0.63
1:C:502:GLY:C	1:C:506:GLN:HG3	2.24	0.63
1:B:44:ARG:CZ	1:B:49:HIS:CD2	2.82	0.63
1:B:1145:LEU:HD22	1:B:1145:LEU:N	2.13	0.63
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.80	0.63
1:B:372:ALA:CB	1:B:374:PHE:CE2	2.73	0.63
1:C:95:THR:HG23	1:C:186:PHE:CD2	2.33	0.63
1:A:1032:CYS:SG	1:A:1064:HIS:CE1	2.92	0.63
1:B:119:ILE:CG1	1:B:128:ILE:CG1	2.62	0.63
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.14	0.63
1:C:110:LEU:HD12	1:C:237:ARG:HH12	1.63	0.63
1:C:200:TYR:CD2	1:C:230:PRO:CA	2.78	0.63
1:C:1029:MET:HE1	1:C:1060:VAL:HG21	1.81	0.63
1:A:332:ILE:HD12	1:A:332:ILE:N	2.12	0.63
1:A:890:ALA:HA	1:C:1046:GLY:HA3	1.80	0.63
1:A:1021:SER:O	1:A:1025:ALA:CA	2.47	0.63
1:B:200:TYR:HE1	1:B:202:LYS:CG	2.11	0.63
1:B:472:ILE:HA	1:B:489:TYR:O	1.99	0.63
1:B:1082:CYS:SG	1:B:1126:CYS:CB	2.87	0.63
1:C:229:LEU:HB3	1:C:231:ILE:HD13	1.80	0.63
1:C:337:PRO:CD	1:C:358:ILE:HD11	2.22	0.63
1:B:117:LEU:HD23	1:B:117:LEU:C	2.24	0.63
1:C:37:TYR:HB3	1:C:223:LEU:CD1	2.28	0.63
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.66	0.63
1:B:270:LEU:HD12	1:B:270:LEU:H	1.64	0.62
1:B:473:TYR:N	1:B:489:TYR:O	2.29	0.62
1:B:537:LYS:O	1:B:551:VAL:HG12	1.97	0.62
1:C:758:SER:HB2	1:C:761:THR:HB	1.80	0.62
1:C:822:LEU:HD11	1:C:1061:VAL:HG21	1.81	0.62
1:A:403:ARG:HG3	1:A:495:TYR:CZ	2.34	0.62
1:A:825:LYS:HE2	1:A:941:THR:O	1.99	0.62
1:B:559:PHE:HB3	1:B:577:ARG:HH21	1.64	0.62
1:B:919:ASN:N	1:B:919:ASN:OD1	2.33	0.62
1:B:986:PRO:N	1:B:987:PRO:CD	2.62	0.62
1:A:964:LYS:O	1:A:965:GLN:C	2.42	0.62
1:B:119:ILE:HG23	1:B:127:VAL:O	2.00	0.62
1:A:107:GLY:HA2	1:A:235:ILE:CG2	2.23	0.62
1:B:96:GLU:OE2	1:B:101:ILE:O	2.17	0.62
1:C:231:ILE:HD12	1:C:231:ILE:N	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:TYR:CE2	1:C:412:PRO:HD3	2.33	0.62
1:C:498:GLN:CG	1:C:499:PRO:HD2	2.29	0.62
1:A:203:ILE:CG2	1:A:227:VAL:HG23	2.29	0.62
1:A:1044:GLY:N	1:A:1064:HIS:ND1	2.47	0.62
1:A:1088:HIS:HB3	1:A:1120:THR:HB	1.82	0.62
1:B:334:ASN:O	1:B:361:CYS:C	2.41	0.62
1:B:726:ILE:CG2	1:B:948:LEU:CG	2.77	0.62
1:B:1039:ARG:NE	1:B:1042:PHE:CD2	2.68	0.62
1:C:105:ILE:HD12	1:C:105:ILE:N	2.15	0.62
1:C:541:PHE:HB3	1:C:552:LEU:HD11	1.80	0.62
1:C:599:THR:CB	1:C:608:VAL:HG12	2.28	0.62
1:A:89:GLY:HA2	1:A:270:LEU:CG	2.29	0.62
1:A:1138:TYR:CE2	1:A:1140:PRO:CA	2.82	0.62
1:B:720:ILE:HD13	1:B:1067:TYR:HA	1.81	0.62
1:C:497:PHE:HD1	1:C:507:PRO:HD3	1.64	0.62
1:A:424:LYS:O	1:A:463:PRO:HA	1.98	0.62
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.15	0.62
1:C:552:LEU:HD22	1:C:587:ILE:CD1	2.27	0.62
1:B:126:VAL:CG2	1:B:172:SER:HB2	2.30	0.62
1:B:1028:LYS:NZ	1:B:1042:PHE:CD1	2.54	0.62
1:C:168:PHE:CZ	1:C:231:ILE:HD11	2.35	0.62
1:C:612:TYR:CB	1:C:615:VAL:HG11	2.27	0.62
1:A:1095:PHE:HB3	1:A:1102:TRP:HZ3	1.65	0.62
1:B:466:ARG:NH1	1:B:468:ILE:HG23	2.14	0.62
1:C:738:CYS:SG	1:C:760:CYS:O	2.58	0.62
1:A:331:ASN:HB3	1:A:580:GLN:HE21	1.63	0.62
1:A:724:THR:CG2	1:A:1063:LEU:HD23	2.26	0.62
1:A:1078:ALA:N	1:A:1102:TRP:CH2	2.68	0.62
1:B:543:PHE:CD2	1:B:576:VAL:HG22	2.34	0.62
1:C:210:ILE:CB	1:C:212:LEU:HD21	2.21	0.62
1:C:673:SER:O	1:C:693:ILE:HG12	2.00	0.62
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.82	0.62
1:A:895:GLN:NE2	1:C:713:ALA:HB2	2.15	0.61
1:B:201:PHE:CE1	1:B:203:ILE:CG1	2.71	0.61
1:B:826:VAL:HG21	1:B:1057:PRO:CG	2.27	0.61
1:C:32:PHE:CE1	1:C:218:GLN:CB	2.83	0.61
1:C:110:LEU:CD1	1:C:237:ARG:HH12	2.13	0.61
1:C:429:PHE:CZ	1:C:431:GLY:C	2.78	0.61
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.34	0.61
1:C:360:ASN:HA	1:C:523:THR:CG2	2.30	0.61
1:C:541:PHE:HE2	1:C:587:ILE:HG21	1.54	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:931:ILE:O	1:C:934:ILE:CG2	2.49	0.61
1:A:726:ILE:HD12	1:A:944:ALA:C	2.24	0.61
1:A:729:VAL:HG21	1:A:1060:VAL:CG2	2.29	0.61
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.79	0.61
1:B:69:HIS:CD2	1:B:77:LYS:HA	2.35	0.61
1:B:365:TYR:CB	1:B:387:LEU:HD12	2.26	0.61
1:B:726:ILE:HD12	1:B:1061:VAL:CG2	2.26	0.61
1:B:1088:HIS:NE2	1:B:1137:VAL:HG21	2.14	0.61
1:A:417:LYS:NZ	1:A:455:LEU:O	2.32	0.61
1:A:620:VAL:HG23	1:A:621:PRO:CD	2.22	0.61
1:B:334:ASN:O	1:B:361:CYS:CA	2.48	0.61
1:B:365:TYR:CD1	1:B:387:LEU:HB3	2.36	0.61
1:C:366:SER:O	1:C:370:ASN:HB3	1.97	0.61
1:A:895:GLN:H	1:A:895:GLN:CD	2.08	0.61
1:A:964:LYS:HB2	1:A:964:LYS:NZ	2.16	0.61
1:A:1081:ILE:HG21	1:A:1135:ASN:CB	2.26	0.61
1:B:322:PRO:CB	1:B:549:THR:CG2	2.78	0.61
1:B:965:GLN:HE21	1:B:965:GLN:HA	1.65	0.61
1:C:102:ARG:HD3	1:C:141:LEU:HD13	1.83	0.61
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.64	0.61
1:C:555:SER:OG	1:C:584:ILE:O	2.17	0.61
1:B:212:LEU:HD13	1:B:214:ARG:N	2.15	0.61
1:B:422:ASN:HD21	1:B:454:ARG:H	1.48	0.61
1:C:48:LEU:HD12	1:C:48:LEU:N	2.14	0.61
1:C:119:ILE:HG12	1:C:127:VAL:C	2.25	0.61
1:C:224:GLU:N	1:C:224:GLU:OE1	2.33	0.61
1:A:817:PHE:HE2	1:A:935:GLN:CG	2.14	0.61
1:B:277:LEU:HD12	1:B:288:ALA:HB2	1.81	0.61
1:B:804:GLN:O	1:B:818:ILE:HG13	2.00	0.61
1:C:90:VAL:N	1:C:270:LEU:CD1	2.63	0.61
1:C:581:THR:O	1:C:582:LEU:HB3	2.00	0.61
1:C:692:ILE:HD12	1:C:692:ILE:N	2.15	0.61
1:A:96:GLU:OE2	1:A:101:ILE:O	2.17	0.61
1:A:474:GLN:OE1	1:A:479:PRO:CB	2.49	0.61
1:B:200:TYR:HH	1:B:202:LYS:HE2	1.64	0.61
1:B:426:PRO:CB	1:B:464:PHE:CE1	2.81	0.61
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.36	0.61
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.06	0.61
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.83	0.61
1:A:992:GLN:HA	1:A:992:GLN:HE21	1.66	0.61
1:B:280:ASN:HB3	1:B:286:THR:HG23	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:VAL:HG12	1:B:599:THR:HG23	1.83	0.61
1:C:591:SER:HB2	1:C:619:GLU:HG2	1.83	0.61
1:A:693:ILE:HD13	1:A:693:ILE:H	1.64	0.60
1:A:1090:PRO:CG	1:A:1093:GLY:O	2.49	0.60
1:B:197:ILE:N	1:B:197:ILE:HD12	2.16	0.60
1:B:1082:CYS:SG	1:B:1132:ILE:CD1	2.89	0.60
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.84	0.60
1:A:107:GLY:N	1:A:235:ILE:HG21	2.14	0.60
1:A:321:GLN:HA	1:A:321:GLN:NE2	2.15	0.60
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.34	0.60
1:A:529:LYS:HG2	1:A:530:SER:O	2.01	0.60
1:B:335:LEU:HD22	1:B:335:LEU:N	2.15	0.60
1:C:599:THR:HB	1:C:608:VAL:CG1	2.31	0.60
1:C:37:TYR:HB3	1:C:223:LEU:HD11	1.84	0.60
1:C:659:SER:HB3	1:C:698:SER:HB3	1.81	0.60
1:C:733:LYS:HD2	1:C:771:ALA:O	2.00	0.60
1:A:336:CYS:N	1:A:361:CYS:HB2	2.17	0.60
1:A:715:PRO:CA	1:A:1071:GLN:O	2.47	0.60
1:A:886:TRP:HB2	1:A:1035:GLY:HA2	1.83	0.60
1:A:1145:LEU:HD23	1:A:1145:LEU:O	2.01	0.60
1:B:318:PHE:CE2	1:B:615:VAL:HG21	2.35	0.60
1:C:168:PHE:CZ	1:C:229:LEU:HD12	2.36	0.60
1:A:33:THR:HB	1:A:58:PHE:CZ	2.36	0.60
1:A:166:CYS:CB	1:A:169:GLU:OE2	2.50	0.60
1:A:546:LEU:HD23	1:A:546:LEU:C	2.26	0.60
1:A:639:GLY:CA	1:A:642:VAL:CG2	2.70	0.60
1:B:365:TYR:CE2	1:B:388:ASN:N	2.70	0.60
1:B:819:GLU:HG2	1:B:1054:GLN:OE1	2.01	0.60
1:B:1090:PRO:HB3	1:B:1093:GLY:O	2.01	0.60
1:C:220:PHE:CE2	1:C:287:ASP:CA	2.82	0.60
1:C:722:VAL:HA	1:C:1064:HIS:O	2.02	0.60
1:A:797:PHE:CD1	1:A:882:ILE:HG21	2.36	0.60
1:A:1032:CYS:HB3	1:A:1051:SER:HB2	1.84	0.60
1:B:44:ARG:O	1:B:279:TYR:CB	2.49	0.60
1:B:69:HIS:NE2	1:B:77:LYS:HD3	2.16	0.60
1:B:541:PHE:CZ	1:B:587:ILE:CD1	2.80	0.60
1:B:743:CYS:O	1:B:977:LEU:HD12	2.00	0.60
1:B:805:ILE:HA	1:B:818:ILE:HD11	1.83	0.60
1:B:909:ILE:HG23	1:B:1036:GLN:HE22	1.64	0.60
1:C:382:VAL:HG21	1:C:515:PHE:HE2	1.67	0.60
1:A:107:GLY:H	1:A:235:ILE:CG2	2.09	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HB3	1:A:592:PHE:HE2	1.54	0.60
1:B:470:THR:HG22	1:B:492:LEU:CD1	2.32	0.60
1:A:985:ASP:CG	1:A:986:PRO:HD2	2.27	0.60
1:A:1043:CYS:HA	1:A:1064:HIS:HE1	1.67	0.60
1:B:33:THR:HA	1:B:58:PHE:CE2	2.35	0.60
1:B:331:ASN:C	1:B:333:THR:N	2.58	0.60
1:B:563:GLN:HG2	1:C:41:LYS:O	2.01	0.60
1:B:584:ILE:HD12	1:B:584:ILE:N	2.17	0.60
1:B:991:VAL:HG23	1:B:992:GLN:OE1	2.02	0.60
1:A:435:ALA:HB1	1:A:510:VAL:HG22	1.83	0.60
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.65	0.60
1:B:719:THR:O	1:B:1068:VAL:HG22	2.02	0.60
1:B:722:VAL:HG11	1:B:934:ILE:HG13	1.83	0.60
1:B:779:GLN:HA	1:B:779:GLN:OE1	2.01	0.60
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.84	0.60
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.67	0.60
1:B:885:GLY:HA2	1:B:901:GLN:HE21	1.66	0.60
1:A:817:PHE:O	1:A:821:LEU:HD13	2.02	0.59
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.37	0.59
1:A:1138:TYR:HE2	1:A:1140:PRO:CB	2.14	0.59
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.84	0.59
1:C:805:ILE:HD11	1:C:1063:LEU:HD12	1.84	0.59
1:C:965:GLN:HG3	1:C:970:PHE:CZ	2.33	0.59
1:A:616:ASN:HB3	1:A:619:GLU:HG2	1.84	0.59
1:A:826:VAL:O	1:A:829:ALA:O	2.20	0.59
1:B:15:CYS:SG	1:B:16:VAL:N	2.75	0.59
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.84	0.59
1:C:55:PHE:HB2	1:C:275:PHE:HE1	1.65	0.59
1:C:220:PHE:CZ	1:C:288:ALA:CA	2.73	0.59
1:C:423:TYR:CE2	1:C:425:LEU:HD21	2.37	0.59
1:C:774:GLN:OE1	1:C:774:GLN:HA	2.01	0.59
1:A:29:THR:O	1:A:62:VAL:HG12	2.02	0.59
1:A:55:PHE:CD1	1:A:275:PHE:CD2	2.90	0.59
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.83	0.59
1:B:56:LEU:CD1	1:B:57:PRO:HD2	2.27	0.59
1:B:91:TYR:HE1	1:B:93:ALA:HB2	1.65	0.59
1:B:338:PHE:HE2	1:B:363:ALA:CB	2.15	0.59
1:B:338:PHE:CE2	1:B:363:ALA:HB1	2.37	0.59
1:B:540:ASN:OD1	1:B:549:THR:CB	2.51	0.59
1:C:314:GLN:O	1:C:314:GLN:HG3	2.01	0.59
1:C:365:TYR:OH	1:C:392:PHE:CZ	2.14	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ASN:O	1:C:449:TYR:CD1	2.55	0.59
1:C:453:TYR:O	1:C:493:GLN:HB3	2.02	0.59
1:C:33:THR:CA	1:C:58:PHE:CD1	2.71	0.59
1:C:33:THR:N	1:C:58:PHE:CD1	2.70	0.59
1:C:106:PHE:HZ	1:C:194:PHE:CD2	2.20	0.59
1:C:330:PRO:HD3	1:C:544:ASN:HD22	1.54	0.59
1:C:765:ARG:HA	1:C:768:THR:HG22	1.83	0.59
1:C:825:LYS:CE	1:C:942:ALA:CB	2.76	0.59
1:A:117:LEU:HD13	1:A:201:PHE:CE2	2.37	0.59
1:A:777:ASN:HD21	1:A:1019:ARG:HA	1.67	0.59
1:B:55:PHE:HB2	1:B:275:PHE:CE2	2.38	0.59
1:B:322:PRO:CB	1:B:549:THR:HG23	2.33	0.59
1:B:564:GLN:NE2	1:B:564:GLN:HA	2.17	0.59
1:C:69:HIS:NE2	1:C:77:LYS:HD3	2.17	0.59
1:C:212:LEU:HD22	1:C:212:LEU:N	2.16	0.59
1:C:544:ASN:CG	1:C:579:PRO:HG3	2.27	0.59
1:C:712:ILE:HD12	1:C:1094:VAL:HG11	1.83	0.59
1:C:738:CYS:SG	1:C:760:CYS:C	2.86	0.59
1:A:353:TRP:CE2	1:A:466:ARG:HB2	2.38	0.59
1:A:552:LEU:HD23	1:A:552:LEU:N	2.18	0.59
1:B:541:PHE:HE2	1:B:587:ILE:HG23	1.64	0.59
1:B:659:SER:HB3	1:B:698:SER:HB3	1.85	0.59
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.85	0.59
1:B:125:ASN:OD1	1:B:172:SER:O	2.19	0.59
1:A:535:LYS:C	1:A:536:ASN:HD22	2.11	0.59
1:A:777:ASN:ND2	1:A:1019:ARG:HA	2.17	0.59
1:B:352:ALA:HA	1:B:466:ARG:NE	2.18	0.59
1:C:86:PHE:CE2	1:C:106:PHE:CE1	2.91	0.59
1:C:503:VAL:HA	1:C:506:GLN:CG	2.33	0.59
1:C:905:ARG:NE	1:C:1050:MET:HE2	2.17	0.59
1:A:203:ILE:CG2	1:A:227:VAL:CG2	2.81	0.59
1:B:44:ARG:HB2	1:B:279:TYR:CE2	2.37	0.59
1:B:197:ILE:CD1	1:B:202:LYS:HD2	2.24	0.59
1:A:331:ASN:HB3	1:A:580:GLN:NE2	2.18	0.58
1:A:718:PHE:HD2	1:A:1109:PHE:CE2	2.21	0.58
1:B:55:PHE:HB2	1:B:275:PHE:HE2	1.68	0.58
1:B:128:ILE:HG22	1:B:129:LYS:N	2.18	0.58
1:B:335:LEU:O	1:B:361:CYS:CB	2.48	0.58
1:B:472:ILE:HD12	1:B:490:PHE:HB2	1.85	0.58
1:C:1004:LEU:O	1:C:1004:LEU:HD23	2.02	0.58
1:A:536:ASN:HD22	1:A:536:ASN:N	2.01	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ILE:CG2	1:A:1135:ASN:CB	2.81	0.58
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.39	0.58
1:B:44:ARG:NH2	1:B:49:HIS:NE2	2.51	0.58
1:B:53:ASP:O	1:B:55:PHE:HD2	1.85	0.58
1:B:546:LEU:CD1	1:B:573:THR:CB	2.81	0.58
1:C:119:ILE:CD1	1:C:128:ILE:CG1	2.80	0.58
1:A:369:TYR:OH	1:A:384:PRO:HB2	2.03	0.58
1:A:1085:GLY:C	1:A:1126:CYS:SG	2.86	0.58
1:B:543:PHE:CB	1:B:576:VAL:CB	2.80	0.58
1:B:1029:MET:HE2	1:B:1062:PHE:HZ	1.69	0.58
1:C:458:LYS:HA	1:C:473:TYR:HE1	1.68	0.58
1:C:718:PHE:CZ	1:C:923:ILE:CG1	2.80	0.58
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.18	0.58
1:A:804:GLN:OE1	1:A:931:ILE:HG22	2.02	0.58
1:B:128:ILE:CG2	1:B:129:LYS:N	2.67	0.58
1:B:546:LEU:HB3	1:B:565:PHE:HE1	1.68	0.58
1:C:318:PHE:HD1	1:C:593:GLY:HA3	1.60	0.58
1:B:245:HIS:HB3	1:B:259:THR:O	2.04	0.58
1:B:365:TYR:CD1	1:B:387:LEU:CB	2.86	0.58
1:B:105:ILE:HG13	1:B:118:LEU:CD1	2.33	0.58
1:B:334:ASN:O	1:B:361:CYS:HA	2.04	0.58
1:B:382:VAL:HA	1:C:984:LEU:HD13	1.84	0.58
1:C:773:GLU:OE2	1:C:1019:ARG:HG3	2.02	0.58
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.36	0.58
1:A:643:PHE:CD2	1:A:655:HIS:CB	2.87	0.58
1:C:326:ILE:HG13	1:C:326:ILE:O	2.03	0.58
1:C:366:SER:O	1:C:370:ASN:HB2	2.02	0.58
1:C:977:LEU:HD21	1:C:1000:ARG:NH1	2.18	0.58
1:A:643:PHE:CE2	1:A:655:HIS:CG	2.92	0.58
1:A:770:ILE:O	1:A:774:GLN:HG2	2.04	0.58
1:A:906:PHE:O	1:A:909:ILE:CG1	2.50	0.58
1:B:422:ASN:HD21	1:B:453:TYR:HA	1.69	0.58
1:A:617:CYS:SG	1:A:644:GLN:CA	2.92	0.58
1:C:426:PRO:CG	1:C:464:PHE:CD2	2.87	0.58
1:C:989:ALA:O	1:C:993:ILE:CG1	2.52	0.58
1:A:166:CYS:CB	1:A:169:GLU:CD	2.77	0.58
1:B:388:ASN:OD1	1:B:527:PRO:HG2	2.04	0.58
1:B:965:GLN:HA	1:B:965:GLN:NE2	2.19	0.58
1:C:534:VAL:CG1	1:C:539:VAL:HG21	2.34	0.58
1:A:332:ILE:H	1:A:332:ILE:CD1	2.16	0.57
1:A:788:ILE:HG13	1:C:699:LEU:HG	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PHE:CD2	1:B:576:VAL:CG2	2.86	0.57
1:B:699:LEU:HD22	1:B:699:LEU:H	1.69	0.57
1:B:737:ASP:N	1:B:737:ASP:OD1	2.35	0.57
1:B:912:THR:HG23	1:B:1106:GLN:OE1	2.03	0.57
1:B:1010:GLN:CB	1:B:1014:ARG:NH1	2.41	0.57
1:C:34:ARG:HG3	1:C:91:TYR:OH	2.04	0.57
1:C:95:THR:OG1	1:C:186:PHE:HB3	2.04	0.57
1:C:1103:PHE:CE1	1:C:1114:ILE:HD13	2.36	0.57
1:A:85:PRO:HG2	1:A:269:TYR:HH	1.67	0.57
1:A:736:VAL:HG21	1:A:858:LEU:HD22	1.86	0.57
1:A:1102:TRP:CB	1:A:1135:ASN:HD21	1.96	0.57
1:B:44:ARG:O	1:B:279:TYR:CG	2.57	0.57
1:B:365:TYR:CG	1:B:387:LEU:CB	2.87	0.57
1:B:1142:GLN:HA	1:B:1142:GLN:NE2	2.18	0.57
1:C:210:ILE:H	1:C:210:ILE:CD1	2.14	0.57
1:C:337:PRO:HD2	1:C:358:ILE:CD1	2.24	0.57
1:C:984:LEU:CG	1:C:988:GLU:HG2	2.33	0.57
1:A:1078:ALA:HB3	1:A:1102:TRP:CH2	2.39	0.57
1:B:805:ILE:HA	1:B:818:ILE:HD12	1.85	0.57
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.85	0.57
1:C:699:LEU:H	1:C:699:LEU:CD2	2.18	0.57
1:C:733:LYS:HB3	1:C:771:ALA:HB1	1.86	0.57
1:A:86:PHE:CD2	1:A:90:VAL:HB	2.40	0.57
1:A:621:PRO:HB2	1:A:637:SER:CB	2.28	0.57
1:A:329:PHE:CD2	1:A:528:LYS:HB3	2.39	0.57
1:A:600:PRO:HG2	1:A:674:TYR:CD1	2.40	0.57
1:A:749:CYS:HA	1:A:993:ILE:HD13	1.85	0.57
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.69	0.57
1:A:890:ALA:HA	1:C:1046:GLY:CA	2.33	0.57
1:B:699:LEU:HD13	1:B:699:LEU:N	2.20	0.57
1:C:1095:PHE:CE1	1:C:1120:THR:HG21	2.39	0.57
1:A:123:ALA:O	1:A:175:PHE:O	2.21	0.57
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.86	0.57
1:A:697:MET:HE3	1:B:869:MET:SD	2.44	0.57
1:A:1021:SER:O	1:A:1025:ALA:CB	2.53	0.57
1:A:1044:GLY:N	1:A:1064:HIS:HD1	2.01	0.57
1:B:91:TYR:HE1	1:B:93:ALA:CB	2.18	0.57
1:B:368:LEU:O	1:B:372:ALA:CB	2.52	0.57
1:B:455:LEU:N	1:B:491:PRO:O	2.37	0.57
1:B:1039:ARG:NH1	1:B:1042:PHE:HE2	1.90	0.57
1:C:86:PHE:CE2	1:C:106:PHE:HE1	2.23	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:N	1:A:186:PHE:HD2	2.02	0.57
1:A:897:PRO:HB2	1:A:900:MET:HG3	1.87	0.57
1:B:119:ILE:CG1	1:B:127:VAL:O	2.53	0.57
1:B:538:CYS:HA	1:B:551:VAL:CG1	2.34	0.57
1:C:782:PHE:CD2	1:C:870:ILE:HG23	2.39	0.57
1:A:825:LYS:HD2	1:A:938:LEU:O	2.04	0.57
1:A:1105:THR:HB	1:A:1111:GLU:O	2.05	0.57
1:B:325:SER:HA	1:B:540:ASN:O	2.04	0.57
1:B:976:VAL:O	1:B:980:ILE:HG22	2.04	0.57
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.04	0.57
1:B:294:ASP:H	1:B:297:SER:HB2	1.70	0.57
1:B:822:LEU:CD2	1:B:1056:ALA:HB2	2.21	0.57
1:B:1029:MET:HE1	1:B:1053:PRO:CB	2.35	0.57
1:C:100:ILE:HG23	1:C:243:ALA:H	1.69	0.57
1:C:185:ASN:ND2	1:C:211:ASN:HD21	2.02	0.57
1:C:552:LEU:CD2	1:C:587:ILE:HD11	2.29	0.57
1:B:658:ASN:HB2	1:B:660:TYR:CE1	2.40	0.57
1:B:821:LEU:HD11	1:B:824:ASN:ND2	2.20	0.57
1:B:1043:CYS:HB2	1:B:1048:HIS:CD2	2.40	0.57
1:B:1140:PRO:O	1:B:1143:PRO:CD	2.50	0.57
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.38	0.57
1:C:401:VAL:HG22	1:C:509:ARG:HA	1.87	0.57
1:C:411:ALA:CA	1:C:425:LEU:HD12	2.35	0.57
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.86	0.57
1:A:394:ASN:HD21	1:B:230:PRO:HB3	1.70	0.56
1:A:1081:ILE:HG13	1:A:1095:PHE:CE2	2.40	0.56
1:A:1101:HIS:HB2	1:A:1103:PHE:CZ	2.40	0.56
1:B:328:ARG:O	1:B:579:PRO:CD	2.52	0.56
1:B:659:SER:HB3	1:B:698:SER:CB	2.35	0.56
1:C:388:ASN:HD22	1:C:388:ASN:N	2.03	0.56
1:C:555:SER:HG	1:C:584:ILE:C	2.11	0.56
1:A:68:ILE:CB	1:A:262:ALA:HA	2.35	0.56
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.34	0.56
1:A:598:ILE:HD12	1:A:598:ILE:N	2.19	0.56
1:A:919:ASN:O	1:A:923:ILE:HG13	2.06	0.56
1:C:434:ILE:N	1:C:434:ILE:HD12	2.20	0.56
1:A:119:ILE:HG23	1:A:127:VAL:O	2.04	0.56
1:A:353:TRP:H	1:A:466:ARG:HD3	1.67	0.56
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.39	0.56
1:A:487:ASN:HA	1:A:489:TYR:HE1	1.70	0.56
1:A:709:ASN:OD1	1:A:709:ASN:N	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:PHE:CD2	1:A:1109:PHE:HE2	2.24	0.56
1:A:731:MET:HG2	1:A:774:GLN:CD	2.30	0.56
1:A:1084:ASP:CB	1:A:1086:LYS:NZ	2.66	0.56
1:B:322:PRO:CD	1:B:549:THR:HG21	2.34	0.56
1:B:365:TYR:CZ	1:B:387:LEU:HB3	2.41	0.56
1:B:543:PHE:CG	1:B:576:VAL:CB	2.89	0.56
1:B:654:GLU:OE1	1:B:654:GLU:HA	2.04	0.56
1:B:980:ILE:HD11	1:B:984:LEU:HD12	1.88	0.56
1:B:1082:CYS:SG	1:B:1132:ILE:HD11	2.45	0.56
1:C:229:LEU:HB3	1:C:231:ILE:CD1	2.36	0.56
1:C:426:PRO:CG	1:C:464:PHE:CE2	2.82	0.56
1:C:942:ALA:HA	1:C:945:LEU:HD12	1.87	0.56
1:C:987:PRO:O	1:C:990:GLU:HB2	2.05	0.56
1:A:408:ARG:O	1:A:414:GLN:NE2	2.38	0.56
1:C:55:PHE:HB3	1:C:275:PHE:CE1	2.38	0.56
1:C:712:ILE:HD13	1:C:714:ILE:HD11	1.87	0.56
1:C:1145:LEU:C	1:C:1145:LEU:HD13	2.31	0.56
1:A:322:PRO:HB3	1:A:539:VAL:CA	2.36	0.56
1:A:331:ASN:OD1	1:A:580:GLN:NE2	2.38	0.56
1:A:697:MET:O	1:A:697:MET:HG2	2.05	0.56
1:B:226:LEU:CD1	1:B:227:VAL:HG13	2.36	0.56
1:C:118:LEU:CD2	1:C:135:PHE:CE1	2.87	0.56
1:C:472:ILE:CG2	1:C:490:PHE:HD1	2.18	0.56
1:C:498:GLN:HG3	1:C:499:PRO:HD2	1.87	0.56
1:C:611:LEU:O	1:C:611:LEU:HD23	2.05	0.56
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.89	0.56
1:A:617:CYS:SG	1:A:644:GLN:HB2	2.46	0.56
1:B:382:VAL:HA	1:C:983:ARG:O	2.06	0.56
1:B:574:ASP:O	1:B:587:ILE:CB	2.51	0.56
1:B:654:GLU:HB3	1:B:693:ILE:HG22	1.88	0.56
1:C:36:VAL:C	1:C:223:LEU:HD21	2.29	0.56
1:A:89:GLY:CA	1:A:270:LEU:H	2.10	0.56
1:A:1145:LEU:HD23	1:A:1145:LEU:C	2.30	0.56
1:B:329:PHE:HA	1:B:579:PRO:HG3	1.78	0.56
1:B:430:THR:HG21	1:C:983:ARG:HH11	1.71	0.56
1:B:546:LEU:CB	1:B:565:PHE:CE1	2.88	0.56
1:B:1094:VAL:HG21	1:C:900:MET:HE1	1.88	0.56
1:C:458:LYS:HE2	1:C:474:GLN:HE21	1.70	0.56
1:C:644:GLN:HA	1:C:644:GLN:HE21	1.68	0.56
1:C:825:LYS:HZ1	1:C:942:ALA:CB	2.06	0.56
1:C:956:ALA:O	1:C:960:ASN:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:PHE:HE1	1:C:1114:ILE:HD12	1.70	0.56
1:A:216:LEU:HD12	1:A:216:LEU:N	2.21	0.56
1:B:85:PRO:O	1:B:269:TYR:CZ	2.57	0.56
1:B:816:SER:H	1:B:819:GLU:HB2	1.70	0.56
1:B:1114:ILE:HG23	1:B:1138:TYR:CD1	2.40	0.56
1:C:471:GLU:O	1:C:491:PRO:CG	2.54	0.56
1:A:552:LEU:CD2	1:A:587:ILE:CD1	2.75	0.56
1:A:707:TYR:CD1	1:A:708:SER:N	2.74	0.56
1:A:1054:GLN:OE1	1:A:1054:GLN:HA	2.05	0.56
1:B:900:MET:HG2	1:B:917:TYR:OH	2.06	0.56
1:B:1115:ILE:O	1:B:1138:TYR:HD1	1.89	0.56
1:A:885:GLY:CA	1:A:901:GLN:CD	2.78	0.56
1:B:226:LEU:HG	1:B:227:VAL:HG22	1.87	0.56
1:B:326:ILE:HG22	1:B:531:THR:OG1	2.05	0.56
1:B:474:GLN:OE1	1:B:479:PRO:CB	2.54	0.56
1:B:599:THR:CG2	1:B:608:VAL:HG11	2.33	0.56
1:C:33:THR:N	1:C:58:PHE:HD1	2.04	0.56
1:A:166:CYS:HB3	1:A:169:GLU:CD	2.30	0.55
1:A:357:ARG:HG3	1:A:396:TYR:CD1	2.41	0.55
1:B:103:GLY:H	1:B:241:LEU:HB2	1.71	0.55
1:B:275:PHE:HE1	1:B:290:ASP:CB	2.18	0.55
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.35	0.55
1:C:123:ALA:O	1:C:175:PHE:O	2.23	0.55
1:C:461:LEU:HD21	1:C:465:GLU:OE1	2.06	0.55
1:C:472:ILE:HA	1:C:491:PRO:HD3	1.88	0.55
1:A:128:ILE:HG22	1:A:129:LYS:N	2.21	0.55
1:A:353:TRP:N	1:A:466:ARG:HD2	2.11	0.55
1:A:888:PHE:CZ	1:A:1034:LEU:HD22	2.41	0.55
1:B:1049:LEU:N	1:B:1049:LEU:HD12	2.21	0.55
1:C:1141:LEU:HD23	1:C:1141:LEU:C	2.31	0.55
1:B:381:GLY:C	1:C:984:LEU:HD13	2.30	0.55
1:B:577:ARG:HD3	1:B:582:LEU:CD2	2.28	0.55
1:B:731:MET:HE1	1:B:1011:GLN:NE2	2.21	0.55
1:C:105:ILE:HG13	1:C:118:LEU:HD12	1.80	0.55
1:C:453:TYR:CD1	1:C:495:TYR:CD1	2.93	0.55
1:A:421:TYR:HB3	1:A:454:ARG:HD2	1.88	0.55
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.88	0.55
1:B:330:PRO:HD3	1:B:579:PRO:HG3	1.88	0.55
1:B:718:PHE:HZ	1:B:923:ILE:CG1	2.18	0.55
1:C:69:HIS:CD2	1:C:77:LYS:HA	2.41	0.55
1:A:87:ASN:ND2	1:A:269:TYR:CE1	2.75	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:CG	1:B:269:TYR:OH	2.52	0.55
1:B:422:ASN:ND2	1:B:454:ARG:H	2.05	0.55
1:B:546:LEU:CD2	1:B:573:THR:HB	2.36	0.55
1:C:417:LYS:O	1:C:421:TYR:HB2	2.06	0.55
1:C:1001:LEU:C	1:C:1001:LEU:HD13	2.30	0.55
1:A:55:PHE:CD1	1:A:275:PHE:CE2	2.95	0.55
1:B:58:PHE:CD1	1:B:290:ASP:HB2	2.42	0.55
1:C:83:VAL:CB	1:C:237:ARG:HH21	2.19	0.55
1:C:309:GLU:OE1	1:C:309:GLU:HA	2.07	0.55
1:A:1081:ILE:HG23	1:A:1133:VAL:O	2.07	0.55
1:B:336:CYS:SG	1:B:362:VAL:N	2.80	0.55
1:B:733:LYS:HD3	1:B:775:ASP:CG	2.31	0.55
1:C:186:PHE:O	1:C:211:ASN:ND2	2.40	0.55
1:A:90:VAL:HG13	1:A:194:PHE:CB	2.36	0.55
1:A:201:PHE:HD1	1:A:202:LYS:N	2.05	0.55
1:A:724:THR:CG2	1:A:1063:LEU:CD2	2.84	0.55
1:A:735:SER:OG	1:A:861:LEU:HD13	2.07	0.55
1:B:37:TYR:CD1	1:B:37:TYR:C	2.85	0.55
1:C:725:GLU:CD	1:C:1028:LYS:HZ3	2.15	0.55
1:A:193:VAL:HG23	1:A:223:LEU:HD13	1.89	0.55
1:B:317:ASN:ND2	1:C:737:ASP:CB	2.69	0.55
1:B:995:ARG:O	1:B:996:LEU:C	2.46	0.55
1:A:403:ARG:HD3	1:A:495:TYR:CE1	2.42	0.55
1:A:1028:LYS:HZ1	1:A:1064:HIS:CE1	2.25	0.55
1:B:716:THR:O	1:B:1109:PHE:CE1	2.60	0.55
1:B:770:ILE:HD13	1:B:1011:GLN:HB3	1.88	0.55
1:C:462:LYS:HE2	1:C:462:LYS:CA	2.19	0.55
1:C:541:PHE:CE2	1:C:587:ILE:CG1	2.91	0.55
1:A:864:LEU:CD1	1:C:665:PRO:HB2	2.37	0.54
1:B:372:ALA:HB1	1:B:374:PHE:CD2	2.37	0.54
1:C:956:ALA:O	1:C:960:ASN:HB3	2.06	0.54
1:A:546:LEU:HD23	1:A:547:THR:N	2.22	0.54
1:A:1091:ARG:NE	1:A:1118:ASP:O	2.41	0.54
1:C:360:ASN:HD22	1:C:523:THR:CG2	2.13	0.54
1:A:965:GLN:O	1:A:966:LEU:C	2.49	0.54
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.85	0.54
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.48	0.54
1:C:290:ASP:O	1:C:297:SER:CB	2.54	0.54
1:A:68:ILE:HD12	1:A:262:ALA:CB	2.38	0.54
1:A:324:GLU:H	1:A:539:VAL:HG12	1.72	0.54
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:NE	1:B:578:ASP:OD2	2.40	0.54
1:B:472:ILE:HD13	1:B:490:PHE:HD1	1.71	0.54
1:B:715:PRO:CA	1:B:1071:GLN:O	2.54	0.54
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.40	0.54
1:A:886:TRP:HB2	1:A:1035:GLY:N	2.23	0.54
1:B:200:TYR:CE1	1:B:202:LYS:CE	2.89	0.54
1:B:962:LEU:HA	1:B:965:GLN:HG2	1.88	0.54
1:C:930:ALA:O	1:C:934:ILE:HG22	2.07	0.54
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.37	0.54
1:B:985:ASP:CB	1:B:987:PRO:HD2	2.38	0.54
1:C:55:PHE:HD2	1:C:275:PHE:HD1	1.45	0.54
1:C:120:VAL:HG21	1:C:157:PHE:HZ	1.71	0.54
1:C:204:TYR:HD1	1:C:225:PRO:HB3	1.70	0.54
1:A:310:LYS:HB2	1:A:600:PRO:C	2.15	0.54
1:A:391:CYS:SG	1:A:544:ASN:HA	2.48	0.54
1:B:613:GLN:HG2	1:C:861:LEU:HD12	1.89	0.54
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.88	0.54
1:C:988:GLU:C	1:C:990:GLU:N	2.62	0.54
1:C:1029:MET:SD	1:C:1033:VAL:HG21	2.48	0.54
1:A:89:GLY:HA3	1:A:270:LEU:CD1	2.32	0.54
1:A:115:GLN:OE1	1:A:130:VAL:HG12	2.08	0.54
1:A:590:CYS:O	1:A:591:SER:C	2.50	0.54
1:A:735:SER:OG	1:A:861:LEU:CD1	2.56	0.54
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.33	0.54
1:B:360:ASN:OD1	1:B:523:THR:HG22	2.07	0.54
1:B:386:LYS:HE2	1:C:982:SER:O	2.07	0.54
1:B:546:LEU:CB	1:B:565:PHE:HE1	2.21	0.54
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.88	0.54
3:C:1305:NAG:O7	3:C:1305:NAG:H3	2.06	0.54
1:A:90:VAL:HG13	1:A:194:PHE:O	2.08	0.54
1:A:229:LEU:HD12	1:A:229:LEU:N	2.23	0.54
1:A:731:MET:CE	1:A:1011:GLN:HE21	2.21	0.54
1:A:927:PHE:O	1:A:927:PHE:HD1	1.91	0.54
1:B:577:ARG:HA	1:B:584:ILE:HA	1.89	0.54
1:B:639:GLY:HA3	1:B:651:ILE:HD12	1.89	0.54
1:C:58:PHE:HD2	1:C:290:ASP:HB2	1.71	0.54
1:C:353:TRP:HE1	1:C:466:ARG:HB3	1.73	0.54
1:C:457:ARG:C	1:C:473:TYR:HE1	2.14	0.54
1:C:1078:ALA:N	1:C:1102:TRP:HH2	2.05	0.54
1:C:1102:TRP:CB	1:C:1135:ASN:OD1	2.46	0.54
1:A:54:LEU:CD1	1:A:54:LEU:H	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:CYS:SG	1:A:644:GLN:CD	2.91	0.54
1:B:360:ASN:H	1:B:524:VAL:HG22	1.73	0.54
1:B:472:ILE:HD13	1:B:490:PHE:CD1	2.42	0.54
1:C:83:VAL:CB	1:C:237:ARG:NH2	2.70	0.54
1:C:329:PHE:O	1:C:580:GLN:HG3	2.08	0.54
1:A:241:LEU:HD12	1:A:241:LEU:C	2.32	0.53
1:A:669:GLY:HA2	1:B:869:MET:HE1	1.90	0.53
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.89	0.53
1:A:886:TRP:HB2	1:A:1035:GLY:H	1.72	0.53
1:B:201:PHE:HE1	1:B:203:ILE:CD1	2.20	0.53
1:B:310:LYS:HE3	1:B:663:ASP:OD1	2.07	0.53
1:B:533:LEU:HD12	1:B:533:LEU:C	2.33	0.53
1:B:718:PHE:CB	1:B:1067:TYR:CZ	2.82	0.53
1:B:802:PHE:HE1	1:B:1052:PHE:CE2	2.26	0.53
1:A:800:PHE:CE2	1:A:927:PHE:HD2	2.27	0.53
1:B:31:SER:OG	1:B:60:SER:O	2.19	0.53
1:C:106:PHE:CZ	1:C:194:PHE:CD2	2.97	0.53
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.90	0.53
1:C:821:LEU:HD21	1:C:939:SER:CB	2.34	0.53
1:A:280:ASN:HB2	1:A:286:THR:HG23	1.89	0.53
1:A:457:ARG:HG3	1:A:459:SER:O	2.09	0.53
1:B:17:ASN:O	1:B:255:SER:HA	2.07	0.53
1:C:36:VAL:HG21	1:C:220:PHE:HE1	1.73	0.53
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.90	0.53
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.90	0.53
1:A:55:PHE:HB3	1:A:275:PHE:HE2	1.70	0.53
1:A:66:HIS:CD2	1:A:68:ILE:CG2	2.92	0.53
1:A:643:PHE:CD2	1:A:655:HIS:HB2	2.43	0.53
1:A:895:GLN:O	1:C:712:ILE:HA	2.09	0.53
1:B:541:PHE:CE2	1:B:587:ILE:CG2	2.85	0.53
1:B:1027:THR:O	1:B:1031:GLU:N	2.33	0.53
1:A:89:GLY:CA	1:A:270:LEU:CG	2.84	0.53
1:A:277:LEU:HD23	1:A:288:ALA:CB	2.39	0.53
1:A:403:ARG:CD	1:A:495:TYR:HE1	2.22	0.53
1:A:1029:MET:N	1:A:1062:PHE:CZ	2.77	0.53
1:A:1043:CYS:CA	1:A:1064:HIS:CE1	2.91	0.53
1:B:718:PHE:CG	1:B:1067:TYR:CE1	2.71	0.53
1:B:1050:MET:O	1:B:1065:VAL:HG23	2.07	0.53
1:C:37:TYR:CD2	1:C:204:TYR:CE2	2.96	0.53
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.44	0.53
1:C:1090:PRO:CB	1:C:1093:GLY:O	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:CD2	1:A:135:PHE:CZ	2.78	0.53
1:A:204:TYR:CD1	1:A:225:PRO:CB	2.92	0.53
1:A:1102:TRP:CE2	1:A:1133:VAL:HG21	2.44	0.53
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.90	0.53
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.44	0.53
1:B:1090:PRO:N	1:B:1095:PHE:HE1	2.07	0.53
1:C:218:GLN:OE1	1:C:218:GLN:N	2.33	0.53
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.13	0.53
1:C:727:LEU:CG	1:C:1028:LYS:HZ2	2.22	0.53
1:A:54:LEU:H	1:A:54:LEU:HD12	1.74	0.53
1:A:67:ALA:HB3	1:A:263:ALA:CB	2.35	0.53
1:A:133:PHE:HE1	1:A:160:TYR:CE1	2.17	0.53
1:B:365:TYR:HE2	1:B:388:ASN:CA	2.22	0.53
1:B:538:CYS:HA	1:B:551:VAL:HG12	1.89	0.53
1:C:185:ASN:ND2	1:C:211:ASN:ND2	2.57	0.53
1:C:230:PRO:HD2	1:C:231:ILE:HD12	1.89	0.53
1:C:546:LEU:HD23	1:C:546:LEU:C	2.34	0.53
1:C:931:ILE:HA	1:C:934:ILE:CG2	2.39	0.53
1:A:203:ILE:HG22	1:A:227:VAL:CG2	2.38	0.53
1:A:1028:LYS:O	1:A:1062:PHE:CE2	2.62	0.53
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.89	0.53
1:A:64:TRP:CE2	1:A:266:TYR:CE2	2.94	0.53
1:A:89:GLY:O	1:A:270:LEU:HD12	2.09	0.53
1:A:729:VAL:HG22	1:A:1025:ALA:CB	2.38	0.53
1:A:886:TRP:HB2	1:A:1035:GLY:CA	2.39	0.53
1:A:1047:TYR:HD1	1:A:1067:TYR:O	1.91	0.53
1:B:825:LYS:HZ2	1:B:945:LEU:HD12	1.73	0.53
1:B:1114:ILE:CG2	1:B:1138:TYR:CE1	2.91	0.53
1:C:223:LEU:HD23	1:C:223:LEU:N	2.24	0.53
1:C:409:GLN:HE21	1:C:409:GLN:H	1.55	0.53
1:C:724:THR:OG1	1:C:934:ILE:HD13	2.09	0.53
1:A:617:CYS:SG	1:A:644:GLN:CB	2.98	0.52
1:A:781:VAL:HA	1:A:1026:ALA:CA	2.37	0.52
1:A:802:PHE:CD2	1:A:882:ILE:HD13	2.44	0.52
1:A:804:GLN:O	1:A:816:SER:HB3	2.09	0.52
1:B:16:VAL:HG13	1:B:158:ARG:NH2	2.24	0.52
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.70	0.52
1:B:665:PRO:HB2	1:C:864:LEU:HD13	1.91	0.52
1:C:516:GLU:OE2	1:C:519:HIS:CE1	2.63	0.52
1:A:329:PHE:CE2	1:A:528:LYS:CG	2.93	0.52
1:A:722:VAL:HA	1:A:1064:HIS:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:HIS:NE2	1:B:77:LYS:HA	2.23	0.52
1:C:800:PHE:CE1	1:C:898:PHE:HE2	2.28	0.52
1:A:314:GLN:HG3	1:A:314:GLN:O	2.09	0.52
1:B:319:ARG:HA	1:B:591:SER:O	2.09	0.52
1:B:328:ARG:NH2	1:B:533:LEU:CB	2.73	0.52
1:B:332:ILE:HG22	1:B:334:ASN:HD21	1.75	0.52
1:B:388:ASN:ND2	1:B:527:PRO:HG2	2.24	0.52
1:B:569:ILE:HB	1:C:47:VAL:HG11	1.91	0.52
1:C:32:PHE:HE1	1:C:218:GLN:CB	2.22	0.52
1:C:727:LEU:HD11	1:C:1028:LYS:HE3	1.90	0.52
1:C:813:SER:O	1:C:868:GLU:OE1	2.28	0.52
1:C:1010:GLN:CD	1:C:1014:ARG:HH12	2.16	0.52
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	1.91	0.52
1:A:1138:TYR:HE2	1:A:1140:PRO:CA	2.21	0.52
1:B:396:TYR:N	1:B:514:SER:O	2.42	0.52
1:B:699:LEU:HD23	1:C:788:ILE:CG1	2.29	0.52
1:B:743:CYS:SG	1:B:750:SER:HA	2.49	0.52
1:B:1081:ILE:HD12	1:B:1133:VAL:HG23	1.90	0.52
1:C:795:LYS:HB3	1:C:797:PHE:HE2	1.73	0.52
1:A:394:ASN:HD21	1:B:230:PRO:HB2	1.74	0.52
1:C:452:LEU:CD2	1:C:492:LEU:HB3	2.39	0.52
1:C:494:SER:OG	1:C:495:TYR:N	2.42	0.52
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.91	0.52
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.91	0.52
1:A:394:ASN:ND2	1:B:230:PRO:HB3	2.24	0.52
1:A:426:PRO:CG	1:A:463:PRO:HB3	2.38	0.52
1:A:669:GLY:CA	1:B:869:MET:HE1	2.40	0.52
1:A:727:LEU:C	1:A:948:LEU:CD2	2.82	0.52
1:A:743:CYS:O	1:A:977:LEU:CD2	2.57	0.52
1:A:1081:ILE:HD12	1:A:1133:VAL:HG23	1.92	0.52
1:A:1138:TYR:CE2	1:A:1140:PRO:CB	2.92	0.52
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.40	0.52
1:B:955:ASN:O	1:B:959:LEU:HD23	2.10	0.52
1:C:194:PHE:HE1	1:C:203:ILE:HD11	1.75	0.52
1:C:1085:GLY:C	1:C:1126:CYS:SG	2.93	0.52
1:A:193:VAL:HG13	1:A:270:LEU:HD21	1.90	0.52
1:A:1033:VAL:HG21	1:A:1053:PRO:HG3	1.91	0.52
1:B:310:LYS:CE	1:B:663:ASP:OD1	2.58	0.52
1:B:976:VAL:HB	1:B:979:ASP:HB3	1.92	0.52
1:C:89:GLY:CA	1:C:270:LEU:HD13	2.39	0.52
1:C:101:ILE:HD12	1:C:101:ILE:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:TYR:CE2	1:C:425:LEU:CD2	2.93	0.52
1:C:710:ASN:O	1:C:1077:THR:HG22	2.10	0.52
1:A:92:PHE:CE1	1:A:94:SER:CB	2.92	0.52
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.25	0.52
1:A:817:PHE:CE2	1:A:935:GLN:HG3	2.35	0.52
1:B:990:GLU:O	1:B:994:ASP:N	2.27	0.52
1:C:37:TYR:CE2	1:C:204:TYR:CE2	2.97	0.52
1:C:87:ASN:ND2	1:C:269:TYR:CE2	2.74	0.52
1:C:353:TRP:CH2	1:C:423:TYR:HA	2.45	0.52
1:C:453:TYR:OH	1:C:493:GLN:NE2	2.43	0.52
1:C:660:TYR:H	1:C:695:TYR:HE2	1.58	0.52
1:C:1054:GLN:OE1	1:C:1054:GLN:HA	2.09	0.52
1:A:800:PHE:HE2	1:A:927:PHE:HD2	1.57	0.52
1:A:825:LYS:CD	1:A:938:LEU:O	2.58	0.52
1:B:804:GLN:OE1	1:B:804:GLN:N	2.42	0.52
1:C:355:ARG:NH2	1:C:396:TYR:CG	2.77	0.52
1:A:800:PHE:CD2	1:A:927:PHE:CD2	2.98	0.52
1:B:665:PRO:CB	1:C:864:LEU:HD13	2.40	0.52
1:B:1145:LEU:CD2	1:B:1145:LEU:H	2.22	0.52
1:C:43:PHE:CD1	1:C:43:PHE:C	2.88	0.52
1:C:180:GLU:HB3	1:C:182:LYS:HE2	1.92	0.52
1:C:543:PHE:CD2	1:C:576:VAL:HG21	2.45	0.52
1:A:278:LYS:HB3	1:A:287:ASP:O	2.10	0.51
1:A:379:CYS:CB	1:A:384:PRO:HD3	2.39	0.51
1:A:973:ILE:HG22	1:A:983:ARG:NH2	2.21	0.51
1:A:1025:ALA:O	1:A:1029:MET:HG2	2.10	0.51
1:B:44:ARG:HB2	1:B:279:TYR:HD2	1.70	0.51
1:B:64:TRP:HD1	1:B:65:PHE:N	2.08	0.51
1:B:275:PHE:HE1	1:B:290:ASP:HB2	1.74	0.51
1:B:539:VAL:C	1:B:549:THR:HG23	2.36	0.51
1:B:823:PHE:CA	1:B:826:VAL:HG12	2.39	0.51
1:C:1080:ALA:C	1:C:1132:ILE:HG13	2.35	0.51
1:A:931:ILE:O	1:A:934:ILE:HG23	2.10	0.51
1:A:988:GLU:O	1:A:991:VAL:CG1	2.57	0.51
1:A:1082:CYS:HB2	1:A:1132:ILE:HD11	1.92	0.51
1:B:472:ILE:CA	1:B:489:TYR:O	2.58	0.51
1:B:1090:PRO:CD	1:B:1095:PHE:CE1	2.86	0.51
1:B:1095:PHE:CZ	1:B:1120:THR:CG2	2.91	0.51
1:B:1105:THR:OG1	1:B:1111:GLU:O	2.28	0.51
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.42	0.51
1:B:1141:LEU:CD2	1:B:1145:LEU:CD2	2.63	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:CA	1:C:523:THR:HG21	2.40	0.51
1:C:461:LEU:CD2	1:C:465:GLU:OE1	2.57	0.51
1:C:577:ARG:HB2	1:C:584:ILE:HD13	1.92	0.51
1:A:407:VAL:HG21	1:A:508:TYR:HD2	1.75	0.51
1:B:164:ASN:OD1	1:B:165:ASN:ND2	2.43	0.51
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.45	0.51
1:B:805:ILE:CA	1:B:818:ILE:HD11	2.40	0.51
1:B:817:PHE:HD1	1:B:817:PHE:C	2.18	0.51
1:B:821:LEU:HD13	1:B:824:ASN:HD22	1.75	0.51
1:B:915:VAL:O	1:B:919:ASN:OD1	2.28	0.51
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.93	0.51
1:C:392:PHE:CE2	1:C:524:VAL:CG1	2.88	0.51
1:C:480:CYS:HA	1:C:483:VAL:HG12	1.90	0.51
1:A:317:ASN:CG	1:A:592:PHE:CZ	2.78	0.51
1:A:931:ILE:O	1:A:934:ILE:CG2	2.59	0.51
1:A:1043:CYS:C	1:A:1064:HIS:ND1	2.66	0.51
1:B:91:TYR:CE1	1:B:93:ALA:CB	2.87	0.51
1:B:200:TYR:C	1:B:200:TYR:CD1	2.88	0.51
1:B:1080:ALA:O	1:B:1132:ILE:CG1	2.59	0.51
1:C:661:GLU:OE1	1:C:661:GLU:N	2.28	0.51
1:A:33:THR:HA	1:A:58:PHE:CE1	2.46	0.51
1:A:773:GLU:OE2	1:A:1019:ARG:CB	2.59	0.51
1:B:107:GLY:H	1:B:235:ILE:HD13	1.75	0.51
1:B:370:ASN:C	1:B:372:ALA:H	2.19	0.51
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.90	0.51
1:C:220:PHE:CE1	1:C:288:ALA:HB3	2.44	0.51
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.43	0.51
1:C:451:TYR:C	1:C:452:LEU:HD12	2.35	0.51
1:A:273:ARG:HH21	1:A:292:ALA:CB	2.24	0.51
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.46	0.51
1:B:647:ALA:HB2	1:C:862:PRO:HG3	1.93	0.51
1:B:795:LYS:HB3	1:B:797:PHE:CE2	2.45	0.51
1:C:330:PRO:N	1:C:544:ASN:HD21	2.08	0.51
1:A:29:THR:O	1:A:62:VAL:HG13	2.10	0.51
1:A:367:VAL:HG23	1:A:368:LEU:CD2	2.41	0.51
1:B:195:LYS:CB	1:B:197:ILE:HD11	2.35	0.51
1:B:277:LEU:CD1	1:B:288:ALA:HB2	2.40	0.51
1:B:542:ASN:CA	1:B:547:THR:HG23	2.41	0.51
1:B:584:ILE:H	1:B:584:ILE:CD1	2.24	0.51
1:B:1011:GLN:HE21	1:B:1011:GLN:CA	2.07	0.51
1:C:497:PHE:CD1	1:C:507:PRO:CD	2.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:TYR:C	1:C:707:TYR:CD1	2.89	0.51
1:C:733:LYS:HB3	1:C:771:ALA:CB	2.40	0.51
1:C:1048:HIS:CE1	1:C:1050:MET:C	2.89	0.51
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.43	0.51
1:A:135:PHE:CD1	1:A:160:TYR:HB3	2.46	0.51
1:A:302:THR:HG21	1:A:315:THR:HA	1.92	0.51
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.75	0.51
1:A:973:ILE:HB	1:A:980:ILE:HD11	1.93	0.51
1:B:515:PHE:CA	1:B:516:GLU:OE1	2.58	0.51
1:B:559:PHE:CG	1:B:584:ILE:HG12	2.46	0.51
1:B:617:CYS:CA	1:B:649:CYS:SG	2.99	0.51
1:B:1040:VAL:HG12	1:B:1041:ASP:OD1	2.11	0.51
1:B:1046:GLY:HA2	1:C:890:ALA:HA	1.93	0.51
1:C:55:PHE:O	1:C:270:LEU:HB3	2.10	0.51
1:C:915:VAL:HG22	1:C:1111:GLU:OE2	2.11	0.51
1:A:471:GLU:O	1:A:491:PRO:HG3	2.11	0.51
1:A:611:LEU:HG	1:A:611:LEU:O	2.09	0.51
1:B:743:CYS:O	1:B:977:LEU:CD1	2.59	0.51
1:B:877:LEU:HD13	1:B:1029:MET:SD	2.51	0.51
1:B:888:PHE:CD1	1:B:888:PHE:C	2.89	0.51
1:B:1054:GLN:HB2	1:B:1061:VAL:O	2.11	0.51
1:C:410:ILE:O	1:C:410:ILE:HG22	2.11	0.51
1:C:551:VAL:HG22	1:C:588:THR:O	2.10	0.51
1:A:663:ASP:N	1:A:695:TYR:OH	2.44	0.51
1:A:976:VAL:CG1	1:A:979:ASP:CB	2.88	0.51
1:A:1088:HIS:CE1	1:A:1122:VAL:HG13	2.38	0.51
1:B:55:PHE:CB	1:B:275:PHE:CE2	2.90	0.51
1:B:328:ARG:NH2	1:B:533:LEU:HB2	2.26	0.51
1:B:368:LEU:O	1:B:372:ALA:HB2	2.10	0.51
1:B:819:GLU:HG3	1:B:1054:GLN:OE1	2.09	0.51
1:B:1062:PHE:HB3	1:B:1064:HIS:CE1	2.46	0.51
1:C:327:VAL:H	1:C:531:THR:CG2	2.23	0.51
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.45	0.51
1:A:141:LEU:N	1:A:241:LEU:HD11	2.26	0.50
1:A:203:ILE:HG21	1:A:227:VAL:CG2	2.41	0.50
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.11	0.50
1:A:741:TYR:CZ	1:A:966:LEU:CD2	2.93	0.50
1:A:1039:ARG:CZ	1:A:1042:PHE:CD2	2.94	0.50
1:B:384:PRO:O	1:B:387:LEU:HG	2.11	0.50
1:B:388:ASN:CG	1:B:527:PRO:HG2	2.36	0.50
1:B:528:LYS:HZ2	1:B:528:LYS:HB3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:PHE:HB3	1:B:1067:TYR:OH	2.10	0.50
1:C:404:GLY:CA	1:C:508:TYR:CD2	2.94	0.50
1:C:610:VAL:O	1:C:651:ILE:HG12	2.11	0.50
1:A:902:MET:HG3	1:A:916:LEU:HD11	1.92	0.50
1:B:815:ARG:CZ	1:B:823:PHE:CG	2.94	0.50
1:C:105:ILE:HD12	1:C:239:GLN:O	2.11	0.50
1:C:336:CYS:HB2	1:C:363:ALA:HB2	1.94	0.50
1:C:977:LEU:CD2	1:C:1000:ARG:HH12	2.23	0.50
1:A:117:LEU:HD13	1:A:201:PHE:CD2	2.46	0.50
1:A:133:PHE:CZ	1:A:160:TYR:CZ	3.00	0.50
1:B:727:LEU:C	1:B:948:LEU:HD21	2.36	0.50
1:C:280:ASN:OD1	1:C:284:THR:N	2.44	0.50
1:C:615:VAL:CG2	1:C:649:CYS:H	2.24	0.50
1:C:654:GLU:OE2	1:C:693:ILE:HG22	2.11	0.50
1:A:712:ILE:HB	1:A:1077:THR:HG22	1.93	0.50
1:A:955:ASN:OD1	1:A:1014:ARG:HD3	2.11	0.50
1:B:699:LEU:H	1:B:699:LEU:HD13	1.76	0.50
1:C:197:ILE:O	1:C:197:ILE:HG13	2.11	0.50
1:C:328:ARG:HB2	1:C:543:PHE:CD1	2.47	0.50
1:A:86:PHE:CD1	1:A:86:PHE:C	2.89	0.50
1:A:106:PHE:CZ	1:A:194:PHE:CD2	2.94	0.50
1:A:903:ALA:CA	1:A:916:LEU:HD13	2.42	0.50
1:A:1029:MET:HA	1:A:1062:PHE:HE2	1.75	0.50
1:B:393:THR:OG1	1:B:522:ALA:HB3	2.11	0.50
1:B:821:LEU:O	1:B:824:ASN:N	2.44	0.50
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.74	0.50
1:C:102:ARG:NE	1:C:141:LEU:HD22	2.26	0.50
1:C:817:PHE:CE1	1:C:935:GLN:HG3	2.46	0.50
1:C:861:LEU:HD22	1:C:861:LEU:H	1.77	0.50
1:A:92:PHE:C	1:A:92:PHE:CD1	2.90	0.50
1:A:864:LEU:HD13	1:C:665:PRO:HB2	1.94	0.50
1:B:119:ILE:HG13	1:B:127:VAL:O	2.11	0.50
1:B:280:ASN:HB3	1:B:286:THR:CG2	2.42	0.50
1:B:962:LEU:O	1:B:965:GLN:HB2	2.12	0.50
1:A:53:ASP:O	1:A:55:PHE:HD2	1.86	0.50
1:A:64:TRP:CD1	1:A:266:TYR:HD2	2.12	0.50
1:A:639:GLY:O	1:A:640:SER:C	2.55	0.50
1:B:226:LEU:HD12	1:B:227:VAL:HG13	1.93	0.50
1:C:203:ILE:CG2	1:C:227:VAL:HG23	2.34	0.50
1:B:64:TRP:HD1	1:B:65:PHE:H	1.58	0.50
1:B:117:LEU:HD23	1:B:117:LEU:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASP:HB3	1:B:293:LEU:HB2	1.93	0.50
1:B:599:THR:CG2	1:B:608:VAL:CG1	2.81	0.50
1:C:92:PHE:CD1	1:C:92:PHE:C	2.90	0.50
1:C:318:PHE:O	1:C:593:GLY:N	2.45	0.50
1:C:390:LEU:HD12	1:C:390:LEU:C	2.37	0.50
1:C:735:SER:HB2	1:C:861:LEU:HD21	1.84	0.50
1:C:1089:PHE:O	1:C:1120:THR:CA	2.60	0.50
1:A:37:TYR:O	1:A:38:TYR:C	2.55	0.50
1:A:97:LYS:N	1:A:186:PHE:CD2	2.79	0.50
1:A:201:PHE:CD1	1:A:202:LYS:N	2.79	0.50
1:A:763:LEU:HD13	1:A:1004:LEU:HB3	1.92	0.50
1:A:950:ASP:OD1	1:A:954:GLN:NE2	2.45	0.50
1:A:988:GLU:OE1	1:A:988:GLU:HA	2.12	0.50
1:A:1043:CYS:HA	1:A:1064:HIS:CE1	2.45	0.50
1:B:59:PHE:CD1	1:B:293:LEU:HD21	2.46	0.50
1:B:321:GLN:H	1:B:321:GLN:CD	2.20	0.50
1:B:659:SER:CB	1:B:698:SER:CB	2.89	0.50
1:B:662:CYS:HB2	1:B:671:CYS:SG	2.51	0.50
1:B:949:GLN:OE1	1:B:949:GLN:HA	2.12	0.50
1:C:119:ILE:CG1	1:C:128:ILE:CB	2.90	0.50
1:C:119:ILE:CG2	1:C:120:VAL:N	2.75	0.50
1:C:541:PHE:CB	1:C:552:LEU:HD11	2.42	0.50
1:C:611:LEU:HD23	1:C:611:LEU:C	2.37	0.50
1:C:716:THR:N	1:C:1071:GLN:O	2.39	0.50
1:C:730:SER:HB2	1:C:774:GLN:CB	2.42	0.50
1:C:1083:HIS:HB3	1:C:1088:HIS:CE1	2.46	0.50
1:A:788:ILE:CG1	1:C:699:LEU:HG	2.42	0.49
1:A:1029:MET:HA	1:A:1062:PHE:CE2	2.47	0.49
1:B:29:THR:HG23	1:B:62:VAL:HG12	1.94	0.49
1:C:643:PHE:HE1	1:C:655:HIS:CD2	2.30	0.49
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.94	0.49
1:A:430:THR:HG21	1:A:517:LEU:HD21	1.94	0.49
1:A:582:LEU:HD22	1:A:582:LEU:N	2.27	0.49
1:A:600:PRO:CG	1:A:674:TYR:CD1	2.96	0.49
1:A:729:VAL:HG22	1:A:1025:ALA:HB1	1.93	0.49
1:B:119:ILE:CG2	1:B:120:VAL:N	2.74	0.49
1:B:193:VAL:CG1	1:B:223:LEU:HD12	2.42	0.49
1:B:273:ARG:HH11	1:B:273:ARG:HG3	1.76	0.49
1:B:533:LEU:HD11	1:B:535:LYS:HG3	1.93	0.49
1:B:989:ALA:HB1	1:B:993:ILE:HD12	1.93	0.49
1:C:659:SER:HB2	1:C:698:SER:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HG22	1:A:259:THR:HG23	1.93	0.49
1:A:662:CYS:HA	1:A:695:TYR:OH	2.12	0.49
1:A:864:LEU:HD12	1:C:667:GLY:HA2	1.94	0.49
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.95	0.49
1:A:1028:LYS:HE3	1:A:1062:PHE:CG	2.47	0.49
1:C:275:PHE:CE2	1:C:290:ASP:OD2	2.65	0.49
1:C:320:VAL:CG2	1:C:591:SER:HB2	2.42	0.49
1:C:365:TYR:N	1:C:365:TYR:CD1	2.81	0.49
1:A:91:TYR:HB2	1:A:270:LEU:HD11	1.95	0.49
1:A:322:PRO:HG3	1:A:549:THR:CG2	2.43	0.49
1:B:86:PHE:C	1:B:86:PHE:CD1	2.90	0.49
1:B:731:MET:H	1:B:774:GLN:CD	2.19	0.49
1:C:368:LEU:HD12	1:C:368:LEU:H	1.76	0.49
1:C:453:TYR:CE2	1:C:493:GLN:CD	2.91	0.49
1:C:726:ILE:HG22	1:C:948:LEU:CG	2.39	0.49
1:C:1033:VAL:HG23	1:C:1062:PHE:HE1	1.77	0.49
1:A:86:PHE:HE2	1:A:90:VAL:CG1	2.24	0.49
1:A:86:PHE:CE2	1:A:90:VAL:HG11	2.42	0.49
1:A:277:LEU:HD23	1:A:288:ALA:HB1	1.94	0.49
1:B:106:PHE:CZ	1:B:194:PHE:CD2	2.94	0.49
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.45	0.49
1:C:105:ILE:HG23	1:C:118:LEU:CD1	2.39	0.49
1:C:360:ASN:HD22	1:C:360:ASN:N	2.10	0.49
1:C:1015:ALA:O	1:C:1019:ARG:N	2.45	0.49
1:A:643:PHE:CD1	1:A:643:PHE:C	2.90	0.49
1:A:922:LEU:HG	1:A:926:GLN:HE21	1.77	0.49
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ2	1.71	0.49
1:B:48:LEU:HD12	1:B:48:LEU:N	2.27	0.49
1:B:817:PHE:C	1:B:817:PHE:CD1	2.88	0.49
1:C:69:HIS:NE2	1:C:77:LYS:HA	2.28	0.49
1:C:472:ILE:O	1:C:472:ILE:HG13	2.13	0.49
1:C:672:ALA:HA	1:C:693:ILE:O	2.13	0.49
1:A:273:ARG:NH2	1:A:292:ALA:CB	2.76	0.49
1:A:743:CYS:SG	1:A:750:SER:CA	3.00	0.49
1:A:800:PHE:CE2	1:A:927:PHE:CD2	3.01	0.49
1:B:101:ILE:HD11	1:B:263:ALA:HB1	1.94	0.49
1:B:342:PHE:CD2	1:B:368:LEU:CD1	2.96	0.49
1:B:639:GLY:CA	1:B:651:ILE:HD12	2.41	0.49
1:B:967:SER:O	1:B:975:SER:HB2	2.12	0.49
1:B:1145:LEU:CD2	1:B:1145:LEU:N	2.75	0.49
1:C:119:ILE:CG1	1:C:128:ILE:CG1	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASN:OD1	1:C:658:ASN:N	2.38	0.49
1:A:33:THR:HA	1:A:58:PHE:CZ	2.47	0.49
1:A:310:LYS:HG3	1:A:664:ILE:CD1	2.31	0.49
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.48	0.49
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.95	0.49
1:B:662:CYS:CB	1:B:671:CYS:SG	3.01	0.49
1:B:1039:ARG:NH2	1:B:1042:PHE:CD2	2.77	0.49
1:C:452:LEU:HG	1:C:494:SER:HA	1.94	0.49
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.46	0.49
1:C:1013:ILE:O	1:C:1017:GLU:HG3	2.12	0.49
1:A:273:ARG:NH2	1:A:292:ALA:HB1	2.27	0.49
1:A:671:CYS:O	1:A:694:ALA:HA	2.13	0.49
1:A:718:PHE:CD1	1:A:718:PHE:C	2.91	0.49
1:B:599:THR:HA	1:B:608:VAL:HG12	1.93	0.49
1:B:720:ILE:CD1	1:B:1067:TYR:HA	2.43	0.49
1:C:119:ILE:CD1	1:C:128:ILE:CG2	2.63	0.49
1:C:422:ASN:O	1:C:461:LEU:HD13	2.13	0.49
1:C:965:GLN:CG	1:C:970:PHE:HZ	2.23	0.49
1:A:289:VAL:HG23	1:A:306:PHE:HE1	1.78	0.49
1:A:480:CYS:SG	1:A:488:CYS:CB	3.01	0.49
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.48	0.49
1:A:805:ILE:O	1:A:816:SER:CB	2.61	0.49
1:B:92:PHE:CE2	1:B:265:TYR:HD2	2.28	0.49
1:B:403:ARG:HG3	1:B:497:PHE:HE1	1.78	0.49
1:C:211:ASN:N	1:C:211:ASN:OD1	2.46	0.49
1:C:341:VAL:CG2	1:C:356:LYS:HD3	2.43	0.49
1:C:360:ASN:N	1:C:523:THR:HG23	2.26	0.49
1:B:119:ILE:HD11	1:B:128:ILE:HG12	1.92	0.48
1:B:753:LEU:HD21	1:B:760:CYS:SG	2.53	0.48
1:B:989:ALA:HB1	1:B:993:ILE:CD1	2.43	0.48
1:C:55:PHE:CD2	1:C:275:PHE:CE1	3.00	0.48
1:C:817:PHE:HE1	1:C:935:GLN:CG	2.25	0.48
1:A:616:ASN:O	1:A:619:GLU:HG2	2.13	0.48
1:A:973:ILE:CG2	1:A:983:ARG:HH21	2.19	0.48
1:B:118:LEU:HB2	1:B:135:PHE:CZ	2.45	0.48
1:B:365:TYR:CZ	1:B:387:LEU:C	2.91	0.48
1:B:521:PRO:CB	1:B:544:ASN:CG	2.84	0.48
1:B:543:PHE:HD2	1:B:576:VAL:HG22	1.78	0.48
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.95	0.48
1:C:231:ILE:H	1:C:231:ILE:CD1	2.23	0.48
1:B:119:ILE:HG13	1:B:128:ILE:CA	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG22	1:B:334:ASN:ND2	2.28	0.48
1:B:383:SER:OG	1:C:985:ASP:HB3	2.12	0.48
1:B:816:SER:OG	1:B:819:GLU:CG	2.61	0.48
1:B:1107:ARG:CZ	1:C:896:ILE:HD11	2.43	0.48
1:C:695:TYR:N	1:C:695:TYR:CD1	2.81	0.48
1:C:795:LYS:HB3	1:C:797:PHE:CE2	2.48	0.48
1:C:821:LEU:CD2	1:C:939:SER:HB3	2.38	0.48
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.49	0.48
1:A:33:THR:CG2	1:A:58:PHE:CD2	2.59	0.48
1:A:119:ILE:CG2	1:A:120:VAL:N	2.77	0.48
1:A:313:TYR:N	1:A:313:TYR:CD1	2.82	0.48
1:A:320:VAL:HG12	1:A:321:GLN:N	2.28	0.48
1:A:695:TYR:CD1	1:A:695:TYR:N	2.81	0.48
1:A:974:SER:OG	1:A:980:ILE:HG12	2.13	0.48
1:B:122:ASN:O	1:B:175:PHE:CE2	2.66	0.48
1:B:200:TYR:CE1	1:B:202:LYS:CG	2.93	0.48
1:B:805:ILE:CG1	1:B:818:ILE:HD11	2.43	0.48
1:C:387:LEU:O	1:C:390:LEU:CD1	2.61	0.48
1:C:472:ILE:CA	1:C:491:PRO:HD3	2.44	0.48
1:C:661:GLU:H	1:C:661:GLU:CD	2.18	0.48
1:C:1067:TYR:CD1	1:C:1067:TYR:C	2.91	0.48
1:A:733:LYS:HE3	1:A:863:PRO:HA	1.94	0.48
1:A:890:ALA:CA	1:C:1046:GLY:HA3	2.43	0.48
1:A:1103:PHE:N	1:A:1103:PHE:CD1	2.81	0.48
1:B:633:TRP:CE3	1:B:636:TYR:O	2.67	0.48
1:B:726:ILE:HG21	1:B:948:LEU:HG	1.95	0.48
1:C:409:GLN:H	1:C:409:GLN:NE2	2.11	0.48
1:C:581:THR:HG21	1:C:583:GLU:CD	2.38	0.48
1:A:782:PHE:HE2	1:A:874:THR:CG2	2.26	0.48
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.44	0.48
1:B:164:ASN:OD1	1:B:165:ASN:OD1	2.32	0.48
1:B:718:PHE:CZ	1:B:923:ILE:CD1	2.88	0.48
1:B:1088:HIS:CD2	1:B:1137:VAL:CG1	2.71	0.48
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.95	0.48
1:C:490:PHE:CZ	1:C:492:LEU:HD23	2.48	0.48
1:C:660:TYR:N	1:C:660:TYR:CD1	2.81	0.48
1:C:710:ASN:O	1:C:1077:THR:N	2.41	0.48
1:C:886:TRP:CD1	1:C:886:TRP:C	2.91	0.48
1:A:743:CYS:C	1:A:977:LEU:CD2	2.87	0.48
1:A:822:LEU:O	1:A:826:VAL:HG23	2.14	0.48
1:B:855:PHE:CD1	1:B:855:PHE:C	2.91	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:PHE:CE1	1:C:434:ILE:HG13	2.45	0.48
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.77	0.48
1:A:96:GLU:OE1	1:A:100:ILE:N	2.46	0.48
1:A:661:GLU:O	1:A:695:TYR:CE2	2.67	0.48
1:B:190:ARG:NE	1:B:207:HIS:CE1	2.76	0.48
1:B:405:ASP:N	1:B:504:GLY:O	2.46	0.48
1:B:543:PHE:CD2	1:B:576:VAL:CB	2.97	0.48
1:C:550:GLY:C	1:C:587:ILE:HG23	2.39	0.48
1:C:661:GLU:O	1:C:695:TYR:OH	2.31	0.48
1:A:96:GLU:HA	1:A:186:PHE:CD2	2.48	0.48
1:A:1067:TYR:C	1:A:1067:TYR:CD1	2.92	0.48
1:B:96:GLU:OE1	1:B:100:ILE:N	2.46	0.48
1:B:914:ASN:OD1	1:B:915:VAL:HG23	2.14	0.48
1:C:85:PRO:HG2	1:C:269:TYR:HH	1.71	0.48
1:C:526:GLY:HA3	1:C:527:PRO:HD2	1.43	0.48
1:A:882:ILE:HG23	1:A:898:PHE:CE1	2.49	0.48
1:B:106:PHE:C	1:B:235:ILE:HD13	2.39	0.48
1:C:32:PHE:HB3	1:C:59:PHE:CE1	2.49	0.48
1:C:1013:ILE:HG22	1:C:1017:GLU:OE2	2.14	0.48
1:A:472:ILE:HG23	1:A:489:TYR:O	2.14	0.47
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.96	0.47
1:B:538:CYS:N	1:B:551:VAL:CG1	2.71	0.47
1:B:763:LEU:HD13	1:B:1004:LEU:HB3	1.96	0.47
1:B:1039:ARG:CZ	1:B:1042:PHE:HD2	2.23	0.47
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.93	0.47
1:C:90:VAL:C	1:C:270:LEU:HD11	2.40	0.47
1:C:458:LYS:HA	1:C:473:TYR:CE1	2.48	0.47
1:A:92:PHE:HE1	1:A:94:SER:CB	2.26	0.47
1:A:104:TRP:O	1:A:118:LEU:CD1	2.55	0.47
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.48	0.47
1:A:643:PHE:CE2	1:A:655:HIS:CB	2.97	0.47
1:A:707:TYR:CD1	1:A:707:TYR:C	2.92	0.47
1:A:791:THR:HG21	1:A:806:LEU:HD11	1.96	0.47
1:A:962:LEU:HD22	1:A:1007:TYR:HB2	1.95	0.47
1:B:44:ARG:O	1:B:279:TYR:HB3	2.14	0.47
1:B:59:PHE:CE1	1:B:293:LEU:HD21	2.49	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CE2	2.49	0.47
1:B:216:LEU:H	1:B:216:LEU:HD12	1.78	0.47
1:B:329:PHE:CG	1:B:330:PRO:CD	2.97	0.47
1:B:353:TRP:HH2	1:B:466:ARG:HB3	1.58	0.47
1:B:659:SER:HB2	1:B:698:SER:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:CG	1:B:1069:PRO:HB3	2.44	0.47
1:B:797:PHE:CD1	1:B:802:PHE:HD2	2.32	0.47
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.95	0.47
1:C:555:SER:OG	1:C:585:LEU:N	2.47	0.47
1:A:741:TYR:CE2	1:A:966:LEU:HD21	2.50	0.47
1:A:799:GLY:O	1:A:924:ALA:HB1	2.13	0.47
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.67	0.47
1:B:185:ASN:HB2	1:B:213:VAL:HG21	1.96	0.47
1:B:365:TYR:OH	1:B:387:LEU:O	2.31	0.47
1:B:1010:GLN:O	1:B:1014:ARG:HG3	2.15	0.47
1:C:126:VAL:HG13	1:C:175:PHE:HZ	1.78	0.47
1:C:220:PHE:CE2	1:C:287:ASP:C	2.92	0.47
1:C:429:PHE:CD1	1:C:431:GLY:N	2.78	0.47
1:C:541:PHE:C	1:C:541:PHE:CD1	2.91	0.47
1:C:581:THR:CG2	1:C:583:GLU:HG3	2.40	0.47
1:C:817:PHE:CD1	1:C:817:PHE:C	2.92	0.47
1:C:868:GLU:OE1	1:C:868:GLU:HA	2.14	0.47
1:C:945:LEU:O	1:C:946:GLY:C	2.57	0.47
1:A:126:VAL:HG13	1:A:175:PHE:CZ	2.49	0.47
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.95	0.47
1:B:466:ARG:HH12	1:B:468:ILE:HG23	1.78	0.47
1:C:366:SER:O	1:C:370:ASN:CA	2.61	0.47
1:C:921:LYS:HA	1:C:921:LYS:HE3	1.91	0.47
1:A:115:GLN:CD	1:A:130:VAL:HG12	2.40	0.47
1:A:128:ILE:CG2	1:A:129:LYS:N	2.77	0.47
1:B:381:GLY:O	1:C:983:ARG:HG2	2.14	0.47
1:C:37:TYR:HA	1:C:223:LEU:HG	1.96	0.47
1:C:317:ASN:HA	1:C:593:GLY:O	2.14	0.47
1:C:729:VAL:HG21	1:C:782:PHE:HE1	1.80	0.47
1:C:733:LYS:HD2	1:C:771:ALA:C	2.40	0.47
1:A:230:PRO:CG	1:C:357:ARG:NH1	2.77	0.47
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.48	0.47
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.55	0.47
1:B:817:PHE:HZ	1:B:935:GLN:NE2	2.10	0.47
1:B:977:LEU:HA	1:B:980:ILE:HG22	1.97	0.47
1:C:748:GLU:CD	1:C:981:LEU:HG	2.40	0.47
1:C:791:THR:CG2	1:C:792:PRO:HD2	2.44	0.47
1:C:977:LEU:HD21	1:C:1000:ARG:HH12	1.78	0.47
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.98	0.47
1:B:331:ASN:OD1	2:H:1:NAG:O5	2.27	0.47
1:B:353:TRP:CZ3	1:B:423:TYR:HD1	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:CD1	1:B:490:PHE:CB	2.86	0.47
1:B:743:CYS:C	1:B:749:CYS:SG	2.97	0.47
1:B:911:VAL:HG21	1:B:1067:TYR:CE2	2.50	0.47
1:B:1116:THR:HG22	1:B:1140:PRO:CD	2.39	0.47
1:B:1141:LEU:HD11	1:C:1141:LEU:HD12	1.95	0.47
1:C:37:TYR:CB	1:C:223:LEU:HG	2.44	0.47
1:C:83:VAL:HB	1:C:237:ARG:NH2	2.29	0.47
1:C:104:TRP:CE3	1:C:104:TRP:N	2.82	0.47
1:C:168:PHE:CD2	1:C:231:ILE:HG13	2.50	0.47
1:C:194:PHE:CD1	1:C:203:ILE:HG13	2.50	0.47
1:C:270:LEU:HD12	1:C:270:LEU:N	2.30	0.47
1:C:377:PHE:HE1	1:C:434:ILE:HD11	1.80	0.47
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.97	0.47
1:C:728:PRO:HB3	1:C:948:LEU:HD22	1.97	0.47
1:C:817:PHE:HD1	1:C:818:ILE:HD13	1.78	0.47
1:C:1086:LYS:HB3	1:C:1122:VAL:HG21	1.96	0.47
1:A:89:GLY:CA	1:A:270:LEU:N	2.53	0.47
1:B:64:TRP:CD1	1:B:65:PHE:N	2.82	0.47
1:B:118:LEU:CD2	1:B:135:PHE:CE1	2.84	0.47
1:B:168:PHE:CE2	1:B:170:TYR:CB	2.92	0.47
1:B:718:PHE:CZ	1:B:923:ILE:HG12	2.50	0.47
1:B:991:VAL:HG23	1:B:992:GLN:CD	2.40	0.47
1:B:1031:GLU:OE2	1:B:1039:ARG:CD	2.61	0.47
1:B:1145:LEU:HD22	1:B:1145:LEU:H	1.76	0.47
1:C:612:TYR:HB2	1:C:615:VAL:CG2	2.44	0.47
1:C:655:HIS:CD2	1:C:655:HIS:C	2.92	0.47
1:A:43:PHE:CE2	1:A:282:ASN:O	2.54	0.47
1:A:86:PHE:CE2	1:A:90:VAL:CG1	2.98	0.47
1:A:96:GLU:CA	1:A:186:PHE:HD2	2.27	0.47
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.50	0.47
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.97	0.47
1:B:204:TYR:CE1	1:B:225:PRO:CB	2.93	0.47
1:B:238:PHE:C	1:B:238:PHE:CD1	2.93	0.47
1:B:699:LEU:CD2	1:C:788:ILE:HG13	2.31	0.47
1:B:795:LYS:HB3	1:B:797:PHE:HE2	1.80	0.47
1:A:664:ILE:HB	1:A:672:ALA:O	2.15	0.47
1:A:1028:LYS:CB	1:A:1062:PHE:CZ	2.97	0.47
1:B:197:ILE:HD13	1:B:202:LYS:CG	2.44	0.47
1:B:336:CYS:HA	1:B:361:CYS:SG	2.55	0.47
1:B:365:TYR:CG	1:B:387:LEU:HD12	2.50	0.47
1:B:396:TYR:OH	1:C:200:TYR:CZ	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PRO:HD2	1:C:231:ILE:CD1	2.44	0.47
1:C:612:TYR:HB2	1:C:615:VAL:HG13	1.80	0.47
1:C:718:PHE:CD1	1:C:718:PHE:C	2.93	0.47
1:A:93:ALA:O	1:A:266:TYR:CD1	2.61	0.46
1:A:403:ARG:CG	1:A:495:TYR:CZ	2.98	0.46
1:A:403:ARG:HG2	1:A:495:TYR:CE1	2.49	0.46
1:A:743:CYS:O	1:A:977:LEU:HD23	2.14	0.46
1:C:414:GLN:HE21	1:C:414:GLN:CA	2.19	0.46
1:A:276:LEU:HD23	1:A:276:LEU:C	2.39	0.46
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.96	0.46
1:A:650:LEU:HD12	1:A:653:ALA:HB3	1.97	0.46
1:B:265:TYR:N	1:B:265:TYR:CD1	2.83	0.46
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.51	0.46
1:B:1049:LEU:HD11	1:B:1067:TYR:HB2	1.98	0.46
1:C:585:LEU:HD23	1:C:585:LEU:N	2.29	0.46
1:C:734:THR:HG21	1:C:1007:TYR:OH	2.16	0.46
1:A:238:PHE:CD1	1:A:238:PHE:C	2.93	0.46
1:A:731:MET:HE3	1:A:1011:GLN:HE21	1.80	0.46
1:B:365:TYR:CE2	1:B:388:ASN:HA	2.46	0.46
1:B:395:VAL:HG22	1:B:515:PHE:HB3	1.96	0.46
1:C:534:VAL:HG11	1:C:539:VAL:HG21	1.97	0.46
1:C:733:LYS:HD2	1:C:771:ALA:HB1	1.97	0.46
1:A:29:THR:HG23	1:A:62:VAL:HG13	1.97	0.46
1:A:119:ILE:HG22	1:A:120:VAL:N	2.30	0.46
1:A:895:GLN:HE22	1:C:713:ALA:HB2	1.81	0.46
1:A:903:ALA:HA	1:A:916:LEU:CD1	2.45	0.46
1:B:91:TYR:O	1:B:91:TYR:HD1	1.99	0.46
1:B:108:THR:OG1	1:B:234:ASN:O	2.33	0.46
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.97	0.46
1:B:866:THR:HG23	1:B:869:MET:H	1.79	0.46
1:C:588:THR:HG22	1:C:589:PRO:CD	2.44	0.46
1:A:141:LEU:HB2	1:A:241:LEU:HD11	1.98	0.46
1:A:164:ASN:OD1	2:F:1:NAG:O5	2.33	0.46
1:A:216:LEU:HD12	1:A:216:LEU:H	1.80	0.46
1:A:328:ARG:HH22	1:A:533:LEU:CA	2.28	0.46
1:A:914:ASN:O	1:A:918:GLU:HG3	2.15	0.46
1:A:1028:LYS:HE3	1:A:1062:PHE:CD1	2.50	0.46
1:B:101:ILE:HG13	1:B:242:LEU:HD13	1.98	0.46
1:B:229:LEU:N	1:B:229:LEU:HD22	2.30	0.46
1:B:336:CYS:SG	1:B:363:ALA:N	2.88	0.46
1:C:392:PHE:HD2	1:C:395:VAL:HG22	1.67	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:PHE:CE1	1:C:587:ILE:CD1	2.85	0.46
1:C:734:THR:CG2	1:C:1011:GLN:HE21	2.29	0.46
1:A:231:ILE:CG2	1:A:233:ILE:H	2.22	0.46
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.51	0.46
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.51	0.46
1:B:388:ASN:HD21	1:B:527:PRO:HG2	1.79	0.46
1:B:805:ILE:HD13	1:B:1052:PHE:CD2	2.51	0.46
1:B:856:ASN:O	1:B:858:LEU:HG	2.16	0.46
1:C:503:VAL:HG22	1:C:506:GLN:OE1	2.16	0.46
1:C:712:ILE:CD1	1:C:714:ILE:HD11	2.45	0.46
1:A:954:GLN:HG2	1:A:1014:ARG:HH22	1.80	0.46
1:B:107:GLY:N	1:B:235:ILE:CD1	2.75	0.46
1:B:107:GLY:H	1:B:235:ILE:CG2	2.29	0.46
1:B:882:ILE:HG23	1:B:898:PHE:HD2	1.78	0.46
1:B:1081:ILE:HD12	1:B:1133:VAL:CG2	2.46	0.46
1:C:326:ILE:HD11	1:C:552:LEU:HD12	1.96	0.46
1:C:429:PHE:CD1	1:C:429:PHE:C	2.93	0.46
1:C:659:SER:C	1:C:660:TYR:CD1	2.94	0.46
1:C:671:CYS:O	1:C:695:TYR:CE1	2.69	0.46
1:C:720:ILE:CD1	1:C:1049:LEU:HD11	2.46	0.46
1:C:1124:GLY:C	1:C:1125:ASN:HD22	2.24	0.46
1:A:329:PHE:CE2	1:A:528:LYS:HB3	2.50	0.46
1:A:411:ALA:HB3	1:A:414:GLN:HE21	1.81	0.46
1:B:265:TYR:N	1:B:265:TYR:HD1	2.13	0.46
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.97	0.46
1:B:365:TYR:CZ	1:B:387:LEU:O	2.69	0.46
1:C:31:SER:O	1:C:59:PHE:HA	2.16	0.46
1:C:374:PHE:CD1	1:C:374:PHE:N	2.83	0.46
1:C:516:GLU:CD	1:C:519:HIS:NE2	2.72	0.46
1:C:974:SER:HB3	1:C:980:ILE:HD11	1.98	0.46
1:A:231:ILE:CG2	1:A:233:ILE:HG23	2.45	0.46
1:A:1030:SER:OG	1:A:1034:LEU:HD12	2.16	0.46
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.44	0.46
1:B:356:LYS:N	1:B:397:ALA:O	2.45	0.46
1:B:411:ALA:HB3	1:B:414:GLN:HG2	1.96	0.46
1:B:538:CYS:CA	1:B:551:VAL:CG1	2.93	0.46
1:B:763:LEU:HD22	1:B:1008:VAL:CG2	2.42	0.46
1:B:784:GLN:HE21	1:B:784:GLN:CA	2.07	0.46
1:B:1110:TYR:CD1	1:B:1110:TYR:C	2.93	0.46
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.55	0.46
1:C:119:ILE:HG13	1:C:127:VAL:C	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:PHE:CD1	1:C:434:ILE:CG1	2.87	0.46
1:C:671:CYS:O	1:C:695:TYR:CD1	2.69	0.46
1:C:720:ILE:HD11	1:C:1049:LEU:HD11	1.98	0.46
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.56	0.46
1:C:817:PHE:HE1	1:C:935:GLN:HG3	1.81	0.46
1:C:1001:LEU:HD13	1:C:1001:LEU:O	2.16	0.46
1:C:1029:MET:O	1:C:1034:LEU:HG	2.16	0.46
1:A:357:ARG:HD2	1:B:230:PRO:HB2	1.97	0.46
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.82	0.46
1:A:864:LEU:HA	1:C:667:GLY:HA2	1.97	0.46
1:B:318:PHE:O	1:B:592:PHE:HA	2.16	0.46
1:B:805:ILE:HG23	1:B:878:LEU:HD11	1.97	0.46
1:B:821:LEU:CD1	1:B:824:ASN:CB	2.87	0.46
1:B:1080:ALA:O	1:B:1132:ILE:HG13	2.15	0.46
1:C:310:LYS:HB2	1:C:600:PRO:O	2.16	0.46
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.31	0.46
1:A:797:PHE:HE1	1:A:882:ILE:HG22	1.77	0.45
1:B:62:VAL:HG21	1:B:266:TYR:HB3	1.97	0.45
1:B:961:THR:C	1:B:965:GLN:HG2	2.37	0.45
1:B:995:ARG:O	1:B:998:THR:N	2.49	0.45
1:C:395:VAL:CG1	1:C:513:LEU:HD11	2.46	0.45
1:A:57:PRO:HB3	1:A:273:ARG:HE	1.80	0.45
1:A:1043:CYS:CB	1:A:1064:HIS:CE1	2.99	0.45
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.97	0.45
1:B:542:ASN:HA	1:B:547:THR:HG23	1.98	0.45
1:B:555:SER:HB3	1:B:584:ILE:O	2.16	0.45
1:B:817:PHE:HD1	1:B:817:PHE:O	1.98	0.45
1:B:1081:ILE:CD1	1:B:1133:VAL:CG2	2.95	0.45
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.49	0.45
1:C:406:GLU:OE1	1:C:406:GLU:N	2.49	0.45
1:C:1004:LEU:HD23	1:C:1004:LEU:C	2.41	0.45
1:C:1103:PHE:CE1	1:C:1114:ILE:CD1	2.89	0.45
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.80	0.45
1:B:382:VAL:CA	1:C:984:LEU:HD13	2.46	0.45
1:B:396:TYR:HE2	1:C:200:TYR:OH	1.78	0.45
1:B:562:PHE:CZ	1:C:225:PRO:HD2	2.51	0.45
1:B:718:PHE:CZ	1:B:923:ILE:CG1	2.99	0.45
1:C:607:GLN:NE2	1:C:674:TYR:CE1	2.85	0.45
1:C:805:ILE:HD11	1:C:1063:LEU:CD1	2.46	0.45
1:A:743:CYS:SG	1:A:750:SER:HA	2.57	0.45
1:A:782:PHE:CE1	1:A:1060:VAL:HG22	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:LEU:HD11	1:C:715:PRO:HG3	1.98	0.45
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.97	0.45
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.82	0.45
1:B:324:GLU:HG3	1:B:539:VAL:CG2	2.46	0.45
1:B:962:LEU:HA	1:B:965:GLN:CG	2.45	0.45
1:C:315:THR:O	1:C:595:VAL:HB	2.15	0.45
1:A:34:ARG:CZ	1:A:217:PRO:HG2	2.46	0.45
1:A:335:LEU:C	1:A:335:LEU:HD12	2.41	0.45
1:A:738:CYS:SG	1:A:760:CYS:O	2.74	0.45
1:A:916:LEU:O	1:A:916:LEU:HD23	2.17	0.45
1:A:976:VAL:CG1	1:A:979:ASP:HB2	2.47	0.45
1:B:324:GLU:HG3	1:B:539:VAL:HG23	1.98	0.45
1:C:269:TYR:CD1	1:C:269:TYR:N	2.83	0.45
1:C:365:TYR:N	1:C:365:TYR:HD1	2.14	0.45
1:C:660:TYR:C	1:C:695:TYR:HE2	2.24	0.45
1:A:135:PHE:HD1	1:A:160:TYR:HB3	1.81	0.45
1:A:193:VAL:CG2	1:A:223:LEU:CD1	2.94	0.45
1:A:201:PHE:CD1	1:A:201:PHE:C	2.93	0.45
1:A:643:PHE:CD2	1:A:655:HIS:HB3	2.51	0.45
1:A:804:GLN:H	1:A:804:GLN:HG2	1.57	0.45
1:B:118:LEU:CD2	1:B:135:PHE:CZ	2.84	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.52	0.45
1:B:1111:GLU:O	1:B:1111:GLU:HG3	2.16	0.45
1:C:136:CYS:SG	1:C:137:ASN:N	2.90	0.45
1:C:781:VAL:HG22	1:C:1026:ALA:CA	2.47	0.45
1:A:367:VAL:HG23	1:A:368:LEU:HD22	1.98	0.45
1:A:403:ARG:CD	1:A:495:TYR:CE1	3.00	0.45
1:A:453:TYR:HE2	1:A:493:GLN:HG2	1.69	0.45
1:A:489:TYR:N	1:A:489:TYR:CD1	2.85	0.45
1:A:738:CYS:SG	1:A:760:CYS:C	3.00	0.45
1:A:741:TYR:CD1	1:A:741:TYR:C	2.94	0.45
1:A:927:PHE:HE1	1:A:931:ILE:CG1	2.30	0.45
1:A:1095:PHE:HE2	1:A:1115:ILE:HD13	1.82	0.45
3:A:1306:NAG:C1	3:A:1306:NAG:C8	2.94	0.45
1:B:539:VAL:O	1:B:549:THR:HA	2.15	0.45
1:B:564:GLN:HE21	1:B:564:GLN:CA	2.22	0.45
1:B:612:TYR:CD2	1:B:620:VAL:HG11	2.51	0.45
1:B:785:VAL:HG12	1:B:888:PHE:HE1	1.82	0.45
1:B:1083:HIS:CE1	1:B:1136:THR:OG1	2.70	0.45
1:C:643:PHE:CE1	1:C:655:HIS:CD2	3.05	0.45
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.52	0.45
1:A:693:ILE:CD1	1:A:693:ILE:H	2.28	0.45
1:B:57:PRO:CB	1:B:273:ARG:NH1	2.60	0.45
1:B:322:PRO:HD3	1:B:549:THR:HG21	1.98	0.45
1:B:818:ILE:HG13	1:B:818:ILE:H	1.57	0.45
1:B:965:GLN:HE21	1:B:965:GLN:CA	2.25	0.45
1:C:312:ILE:HD11	1:C:596:SER:HB3	1.99	0.45
1:C:990:GLU:OE1	1:C:990:GLU:HA	2.17	0.45
1:A:211:ASN:ND2	1:A:211:ASN:O	2.50	0.45
1:A:954:GLN:CG	1:A:1014:ARG:HH22	2.30	0.45
1:B:126:VAL:CG1	1:B:175:PHE:CZ	2.99	0.45
1:B:334:ASN:CB	1:B:361:CYS:HA	2.45	0.45
1:B:718:PHE:CB	1:B:1067:TYR:OH	2.64	0.45
1:B:1080:ALA:O	1:B:1132:ILE:HG12	2.17	0.45
1:A:90:VAL:HG13	1:A:90:VAL:O	2.16	0.45
1:A:577:ARG:NH2	1:A:582:LEU:HD12	2.32	0.45
1:A:728:PRO:N	1:A:948:LEU:CD2	2.79	0.45
1:A:784:GLN:HE22	1:A:1030:SER:HB2	1.78	0.45
1:A:945:LEU:O	1:A:949:GLN:CB	2.64	0.45
1:A:1096:VAL:HG23	1:A:1096:VAL:O	2.17	0.45
1:B:92:PHE:HZ	1:B:265:TYR:CD2	2.31	0.45
1:B:330:PRO:N	1:B:579:PRO:HG2	2.26	0.45
1:B:821:LEU:O	1:B:824:ASN:CB	2.61	0.45
1:C:226:LEU:CG	1:C:227:VAL:HG13	2.43	0.45
1:A:675:GLN:HE21	1:A:675:GLN:CA	2.23	0.44
1:A:794:ILE:HG22	1:A:796:ASP:H	1.82	0.44
1:A:1028:LYS:C	1:A:1062:PHE:CZ	2.95	0.44
1:B:330:PRO:N	1:B:579:PRO:CG	2.80	0.44
1:B:633:TRP:HE3	1:B:636:TYR:O	2.00	0.44
1:B:1039:ARG:NE	1:B:1042:PHE:HD2	2.14	0.44
1:B:1048:HIS:NE2	1:B:1051:SER:OG	2.43	0.44
1:C:186:PHE:O	1:C:211:ASN:CG	2.59	0.44
1:C:326:ILE:HG21	1:C:534:VAL:CG1	2.46	0.44
1:C:409:GLN:HG2	1:C:416:GLY:HA3	1.99	0.44
1:C:720:ILE:HD12	1:C:1049:LEU:HD12	1.99	0.44
1:C:931:ILE:HA	1:C:934:ILE:HG22	1.98	0.44
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.51	0.44
1:A:101:ILE:HG13	1:A:242:LEU:HD13	1.98	0.44
1:A:612:TYR:CB	1:A:615:VAL:HG22	2.47	0.44
1:A:825:LYS:HE2	1:A:941:THR:C	2.41	0.44
1:A:1028:LYS:HB3	1:A:1062:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ARG:HG2	1:B:207:HIS:CE1	2.52	0.44
1:B:541:PHE:C	1:B:541:PHE:CD1	2.95	0.44
1:B:866:THR:O	1:B:869:MET:N	2.50	0.44
1:C:86:PHE:CD2	1:C:106:PHE:HE1	2.35	0.44
1:C:91:TYR:CD1	1:C:91:TYR:C	2.95	0.44
1:C:131:CYS:HG	1:C:166:CYS:CB	2.28	0.44
1:C:555:SER:OG	1:C:585:LEU:CA	2.66	0.44
1:C:825:LYS:NZ	1:C:942:ALA:CB	2.60	0.44
1:C:1089:PHE:HB2	1:C:1121:PHE:CE1	2.52	0.44
1:A:309:GLU:H	1:A:309:GLU:CD	2.24	0.44
1:A:457:ARG:CG	1:A:459:SER:O	2.65	0.44
1:A:878:LEU:HD23	1:A:878:LEU:C	2.41	0.44
1:A:896:ILE:CG2	1:A:897:PRO:HD2	2.46	0.44
1:A:992:GLN:HE21	1:A:992:GLN:CA	2.30	0.44
1:B:48:LEU:HB3	1:B:276:LEU:HD21	1.99	0.44
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.52	0.44
1:B:240:THR:CG2	1:B:241:LEU:N	2.80	0.44
1:B:276:LEU:CD1	1:B:304:LYS:HA	2.45	0.44
1:B:823:PHE:O	1:B:827:THR:CG2	2.43	0.44
1:B:1097:SER:HB3	1:B:1102:TRP:CG	2.53	0.44
1:A:204:TYR:HD1	1:A:225:PRO:N	2.15	0.44
1:A:560:LEU:HD13	1:A:562:PHE:HE1	1.82	0.44
1:A:962:LEU:HD12	1:A:962:LEU:C	2.42	0.44
1:B:730:SER:HA	1:B:774:GLN:OE1	2.18	0.44
1:B:1027:THR:O	1:B:1031:GLU:CB	2.65	0.44
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	3.00	0.44
1:C:83:VAL:HB	1:C:237:ARG:HH21	1.81	0.44
1:C:116:SER:HA	1:C:233:ILE:HD11	1.98	0.44
1:C:377:PHE:CE1	1:C:434:ILE:CG1	3.01	0.44
1:C:660:TYR:N	1:C:695:TYR:CE2	2.83	0.44
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.98	0.44
1:C:805:ILE:CG2	1:C:878:LEU:HD13	2.48	0.44
1:A:289:VAL:HG23	1:A:306:PHE:CE1	2.53	0.44
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.28	0.44
1:A:488:CYS:C	1:A:489:TYR:CD1	2.95	0.44
1:A:541:PHE:O	1:A:541:PHE:CD1	2.71	0.44
1:A:565:PHE:N	1:A:565:PHE:CD1	2.85	0.44
1:B:123:ALA:HB1	1:B:176:LEU:HD23	1.99	0.44
1:B:131:CYS:HG	1:B:166:CYS:CB	2.31	0.44
1:B:367:VAL:O	1:B:370:ASN:CG	2.61	0.44
1:B:559:PHE:HB3	1:B:577:ARG:NH2	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:HE1	1:C:203:ILE:CD1	2.29	0.44
1:A:96:GLU:CA	1:A:186:PHE:CD2	2.99	0.44
1:A:422:ASN:HD21	1:A:454:ARG:H	1.65	0.44
1:A:743:CYS:O	1:A:977:LEU:HD21	2.18	0.44
1:C:275:PHE:HE2	1:C:290:ASP:OD2	2.01	0.44
1:C:770:ILE:CD1	1:C:1015:ALA:HB2	2.47	0.44
1:A:115:GLN:OE1	1:A:130:VAL:CG1	2.66	0.44
1:A:326:ILE:HG21	1:A:534:VAL:CG2	2.43	0.44
1:A:900:MET:HE3	1:C:1079:PRO:HA	1.99	0.44
1:A:1047:TYR:O	1:A:1066:THR:HA	2.17	0.44
1:B:44:ARG:O	1:B:279:TYR:CD2	2.70	0.44
1:B:291:CYS:O	1:B:298:GLU:HA	2.18	0.44
1:B:726:ILE:HD13	1:B:1061:VAL:HG13	2.00	0.44
1:B:805:ILE:HG23	1:B:878:LEU:CD1	2.48	0.44
1:B:1080:ALA:HB3	1:B:1132:ILE:HG13	2.00	0.44
1:C:105:ILE:HG23	1:C:118:LEU:HB2	1.99	0.44
1:C:410:ILE:HD12	1:C:423:TYR:HD2	1.83	0.44
1:C:552:LEU:HD21	1:C:587:ILE:CD1	2.43	0.44
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.48	0.44
1:A:309:GLU:OE1	1:A:309:GLU:N	2.39	0.44
1:A:600:PRO:CD	1:A:692:ILE:HD11	2.43	0.44
1:A:716:THR:N	1:A:1071:GLN:O	2.50	0.44
1:A:817:PHE:HE2	1:A:935:GLN:CD	2.25	0.44
1:B:54:LEU:HD12	1:B:54:LEU:H	1.83	0.44
1:B:396:TYR:OH	1:C:200:TYR:CE2	2.70	0.44
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.99	0.44
1:B:714:ILE:HG23	1:B:1107:ARG:O	2.18	0.44
1:C:200:TYR:HD2	1:C:230:PRO:CA	2.07	0.44
1:C:309:GLU:O	1:C:313:TYR:OH	2.24	0.44
1:C:318:PHE:N	1:C:593:GLY:O	2.51	0.44
1:C:424:LYS:O	1:C:463:PRO:HA	2.18	0.44
1:C:472:ILE:HG22	1:C:490:PHE:CA	2.29	0.44
1:C:491:PRO:HG2	1:C:492:LEU:HD22	2.00	0.44
1:C:949:GLN:OE1	1:C:949:GLN:HA	2.17	0.44
1:A:16:VAL:HG13	1:A:158:ARG:NH2	2.33	0.44
1:A:36:VAL:HG21	1:A:220:PHE:CE1	2.53	0.44
1:A:84:LEU:O	1:A:237:ARG:HB2	2.18	0.44
1:A:299:THR:HA	1:A:315:THR:HG21	1.98	0.44
1:A:710:ASN:O	1:A:1076:THR:HG23	2.18	0.44
1:A:781:VAL:HA	1:A:1026:ALA:CB	2.47	0.44
1:A:819:GLU:OE2	1:A:1054:GLN:OE1	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD13	1:C:1141:LEU:HD11	2.00	0.44
1:B:30:ASN:HA	1:B:61:ASN:HA	2.00	0.44
1:B:107:GLY:CA	1:B:235:ILE:HG12	2.48	0.44
1:B:454:ARG:CA	1:B:491:PRO:O	2.56	0.44
1:B:532:ASN:OD1	1:B:533:LEU:N	2.51	0.44
1:B:644:GLN:OE1	1:B:645:THR:N	2.51	0.44
1:B:801:ASN:ND2	3:B:1308:NAG:H83	2.33	0.44
1:C:368:LEU:HD12	1:C:368:LEU:N	2.33	0.44
1:C:735:SER:CB	1:C:861:LEU:CD2	2.77	0.44
1:C:782:PHE:CZ	1:C:1060:VAL:HB	2.52	0.44
1:A:472:ILE:HA	1:A:491:PRO:CD	2.48	0.43
1:A:612:TYR:CB	1:A:615:VAL:CG2	2.95	0.43
1:A:730:SER:HA	1:A:774:GLN:NE2	2.32	0.43
1:B:986:PRO:HA	1:B:989:ALA:CB	2.42	0.43
1:C:365:TYR:HH	1:C:392:PHE:HZ	0.58	0.43
1:A:710:ASN:O	1:A:1076:THR:HA	2.17	0.43
1:A:752:LEU:HD12	1:A:993:ILE:CG2	2.48	0.43
1:A:779:GLN:HE21	1:A:864:LEU:HD23	1.83	0.43
1:A:962:LEU:O	1:A:965:GLN:HB2	2.17	0.43
1:B:470:THR:O	1:B:490:PHE:CD1	2.63	0.43
1:B:731:MET:CG	1:B:774:GLN:NE2	2.81	0.43
1:B:866:THR:O	1:B:867:ASP:C	2.60	0.43
1:A:105:ILE:O	1:A:238:PHE:HB2	2.17	0.43
1:A:278:LYS:CB	1:A:306:PHE:HE2	2.13	0.43
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.30	0.43
1:A:409:GLN:NE2	1:A:418:ILE:HG22	2.33	0.43
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.99	0.43
1:B:804:GLN:HA	1:B:817:PHE:HB3	2.00	0.43
1:B:882:ILE:HG23	1:B:898:PHE:CE2	2.52	0.43
1:B:1078:ALA:CB	1:B:1102:TRP:CH2	3.00	0.43
1:C:220:PHE:CE1	1:C:288:ALA:CB	2.99	0.43
1:C:360:ASN:ND2	1:C:360:ASN:N	2.65	0.43
1:C:943:SER:O	1:C:944:ALA:C	2.60	0.43
1:C:988:GLU:O	1:C:989:ALA:C	2.61	0.43
1:A:29:THR:HG23	1:A:62:VAL:CG1	2.47	0.43
1:A:56:LEU:HD12	1:A:57:PRO:CD	2.47	0.43
1:A:299:THR:HA	1:A:315:THR:CG2	2.48	0.43
1:A:719:THR:HG23	1:A:1070:ALA:HB2	2.01	0.43
1:A:882:ILE:HG23	1:A:898:PHE:CD1	2.53	0.43
1:B:365:TYR:CE2	1:B:388:ASN:CA	3.02	0.43
1:B:1078:ALA:HB3	1:B:1102:TRP:CH2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:PHE:O	1:C:229:LEU:O	2.35	0.43
1:C:216:LEU:HD12	1:C:216:LEU:O	2.18	0.43
1:C:360:ASN:CA	1:C:523:THR:CG2	2.97	0.43
1:A:68:ILE:CG1	1:A:262:ALA:HA	2.48	0.43
1:A:231:ILE:HG23	1:A:233:ILE:HG23	2.01	0.43
1:A:726:ILE:CG2	1:A:948:LEU:HD12	2.45	0.43
1:A:817:PHE:CE2	1:A:935:GLN:CD	2.96	0.43
1:A:1138:TYR:HE2	1:A:1140:PRO:HA	1.78	0.43
1:A:1141:LEU:CD1	1:C:1141:LEU:HD11	2.47	0.43
1:B:126:VAL:HG23	1:B:126:VAL:O	2.18	0.43
1:B:534:VAL:HG12	1:B:552:LEU:HD12	2.00	0.43
1:B:785:VAL:HG12	1:B:888:PHE:CE1	2.53	0.43
1:C:97:LYS:H	1:C:186:PHE:HD1	1.67	0.43
1:C:100:ILE:HG23	1:C:243:ALA:N	2.31	0.43
1:C:168:PHE:CG	1:C:231:ILE:HG12	2.53	0.43
1:C:317:ASN:OD1	1:C:317:ASN:N	2.52	0.43
1:C:655:HIS:CB	1:C:694:ALA:O	2.53	0.43
1:C:726:ILE:HG21	1:C:948:LEU:HG	1.99	0.43
1:A:282:ASN:HD22	3:A:1308:NAG:C7	2.30	0.43
1:A:896:ILE:HG22	1:A:897:PRO:CD	2.46	0.43
1:B:471:GLU:O	1:B:491:PRO:CD	2.67	0.43
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.34	0.43
1:B:578:ASP:O	1:B:582:LEU:HA	2.19	0.43
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.54	0.43
1:B:1110:TYR:CD1	1:B:1111:GLU:N	2.87	0.43
1:C:99:ASN:N	1:C:99:ASN:ND2	2.64	0.43
1:C:230:PRO:CD	1:C:231:ILE:HD12	2.48	0.43
1:C:360:ASN:N	1:C:523:THR:CG2	2.78	0.43
1:B:18:LEU:HA	1:B:255:SER:O	2.18	0.43
1:B:1049:LEU:N	1:B:1049:LEU:CD1	2.82	0.43
1:C:44:ARG:O	1:C:279:TYR:HB3	2.19	0.43
1:C:326:ILE:HD13	1:C:534:VAL:HG12	2.01	0.43
1:C:353:TRP:HD1	1:C:353:TRP:O	2.01	0.43
1:C:735:SER:O	1:C:859:THR:O	2.37	0.43
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.32	0.43
1:C:977:LEU:CG	1:C:1000:ARG:NH1	2.74	0.43
1:C:1116:THR:HA	1:C:1138:TYR:O	2.18	0.43
1:A:66:HIS:CD2	1:A:68:ILE:HG22	2.54	0.43
1:A:200:TYR:HE2	1:C:394:ASN:CG	2.27	0.43
1:A:353:TRP:CZ2	1:A:465:GLU:O	2.57	0.43
1:A:641:ASN:CG	1:A:653:ALA:N	2.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.65	0.43
1:A:914:ASN:OD1	1:A:914:ASN:N	2.51	0.43
1:C:354:ASN:HB3	1:C:399:SER:HB2	2.01	0.43
1:C:643:PHE:CE1	1:C:655:HIS:HB3	2.53	0.43
1:C:1076:THR:OG1	1:C:1097:SER:OG	2.34	0.43
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.83	0.43
1:B:336:CYS:O	1:B:338:PHE:N	2.52	0.43
1:B:472:ILE:HD13	1:B:490:PHE:CB	2.49	0.43
1:B:916:LEU:HD12	1:B:923:ILE:HD12	2.01	0.43
1:C:471:GLU:C	1:C:491:PRO:HD3	2.44	0.43
1:C:605:SER:HG	1:C:607:GLN:HG2	1.84	0.43
1:A:35:GLY:HA3	1:A:91:TYR:CE1	2.53	0.43
1:A:235:ILE:HD12	1:A:235:ILE:N	2.30	0.43
1:A:302:THR:HG21	1:A:315:THR:CA	2.49	0.43
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.82	0.43
1:B:44:ARG:CB	1:B:47:VAL:CG2	2.90	0.43
1:B:553:THR:O	1:B:586:ASP:N	2.52	0.43
1:C:100:ILE:CG2	1:C:243:ALA:H	2.32	0.43
1:C:119:ILE:HG12	1:C:128:ILE:CB	2.49	0.43
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.83	0.43
1:C:753:LEU:HD12	1:C:753:LEU:HA	1.82	0.43
1:C:984:LEU:CG	1:C:988:GLU:CG	2.94	0.43
1:A:90:VAL:HG22	1:A:194:PHE:HD2	1.84	0.42
1:B:538:CYS:HA	1:B:551:VAL:HG13	2.00	0.42
1:B:823:PHE:CA	1:B:826:VAL:CG1	2.84	0.42
1:C:192:PHE:HA	1:C:204:TYR:O	2.19	0.42
1:C:382:VAL:HG13	1:C:390:LEU:HD21	2.00	0.42
1:A:91:TYR:HE1	1:A:223:LEU:HD11	1.82	0.42
1:A:92:PHE:CE1	1:A:104:TRP:HZ2	2.37	0.42
1:A:192:PHE:HA	1:A:204:TYR:O	2.19	0.42
1:A:501:ASN:N	1:A:501:ASN:ND2	2.66	0.42
1:A:1078:ALA:CB	1:A:1102:TRP:CH2	3.02	0.42
1:B:200:TYR:CZ	1:B:202:LYS:CE	2.95	0.42
1:B:368:LEU:O	1:B:372:ALA:HB3	2.18	0.42
1:C:210:ILE:CB	1:C:212:LEU:CD2	2.91	0.42
1:C:1145:LEU:HD13	1:C:1145:LEU:O	2.19	0.42
1:A:353:TRP:CE2	1:A:466:ARG:HD3	2.54	0.42
1:A:782:PHE:CE2	1:A:874:THR:CG2	3.02	0.42
1:A:996:LEU:O	1:A:1000:ARG:N	2.44	0.42
1:A:1013:ILE:HD13	1:B:1012:LEU:HB3	2.02	0.42
1:A:1091:ARG:HG3	1:A:1119:ASN:C	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:VAL:O	1:B:17:ASN:OD1	2.37	0.42
1:B:103:GLY:HA3	1:B:241:LEU:HD13	2.01	0.42
1:B:140:PHE:CE1	1:B:244:LEU:HD12	2.54	0.42
1:B:430:THR:HG21	1:C:983:ARG:NH1	2.33	0.42
1:C:238:PHE:HZ	1:C:267:VAL:HG21	1.84	0.42
1:C:365:TYR:CD2	1:C:387:LEU:HD13	2.54	0.42
1:A:208:THR:HA	1:A:209:PRO:HD3	1.88	0.42
1:A:781:VAL:HG13	1:A:1029:MET:HG2	1.99	0.42
1:A:886:TRP:HE3	1:A:886:TRP:O	2.02	0.42
1:B:89:GLY:CA	1:B:270:LEU:HD13	2.50	0.42
1:B:91:TYR:CD1	1:B:91:TYR:C	2.97	0.42
1:B:335:LEU:N	1:B:335:LEU:CD2	2.81	0.42
1:B:916:LEU:CD1	1:B:923:ILE:HD12	2.49	0.42
1:C:195:LYS:HD2	1:C:204:TYR:CE2	2.54	0.42
1:C:245:HIS:HB3	1:C:259:THR:O	2.19	0.42
1:C:355:ARG:HA	1:C:397:ALA:O	2.19	0.42
1:C:856:ASN:OD1	1:C:966:LEU:CD1	2.61	0.42
1:C:878:LEU:HD21	1:C:1053:PRO:HD2	1.99	0.42
1:A:53:ASP:O	1:A:54:LEU:C	2.61	0.42
1:A:1081:ILE:CG1	1:A:1095:PHE:CE2	3.02	0.42
1:B:350:VAL:HG13	1:B:422:ASN:ND2	2.34	0.42
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.01	0.42
1:B:1114:ILE:HD12	1:B:1114:ILE:N	2.34	0.42
1:C:378:LYS:HG3	1:C:433:VAL:HG12	2.01	0.42
1:C:659:SER:HB3	1:C:698:SER:CB	2.49	0.42
1:C:825:LYS:HE3	1:C:942:ALA:HB2	1.96	0.42
1:A:201:PHE:HD1	1:A:201:PHE:C	2.26	0.42
1:A:437:ASN:OD1	1:A:438:SER:N	2.52	0.42
1:A:1047:TYR:CD1	1:A:1047:TYR:N	2.84	0.42
1:B:36:VAL:HG21	1:B:288:ALA:HB3	2.02	0.42
1:B:36:VAL:HG13	1:B:277:LEU:HD11	2.00	0.42
1:B:275:PHE:CE1	1:B:290:ASP:CA	3.02	0.42
1:B:367:VAL:O	1:B:370:ASN:OD1	2.36	0.42
1:B:805:ILE:HG22	1:B:878:LEU:HD13	2.01	0.42
1:C:409:GLN:NE2	1:C:409:GLN:N	2.68	0.42
1:C:472:ILE:CB	1:C:490:PHE:HA	2.48	0.42
1:A:375:SER:OG	1:A:435:ALA:O	2.36	0.42
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.80	0.42
1:A:1095:PHE:HD2	1:A:1102:TRP:HE3	1.68	0.42
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.01	0.42
1:B:801:ASN:HD22	3:B:1308:NAG:H83	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:OE1	1:C:516:GLU:HA	2.19	0.42
1:C:612:TYR:CG	1:C:615:VAL:HG11	2.54	0.42
1:A:317:ASN:HD21	1:B:737:ASP:HB3	1.85	0.42
1:A:961:THR:O	1:A:965:GLN:HG2	2.20	0.42
1:B:273:ARG:NH1	1:B:273:ARG:HG3	2.34	0.42
1:B:884:SER:OG	1:B:888:PHE:HB3	2.20	0.42
1:C:99:ASN:N	1:C:99:ASN:HD22	2.17	0.42
1:C:350:VAL:CG1	1:C:422:ASN:HB2	2.48	0.42
1:C:534:VAL:HG13	1:C:539:VAL:HG21	2.00	0.42
1:C:615:VAL:HG23	1:C:649:CYS:H	1.85	0.42
1:C:692:ILE:H	1:C:692:ILE:CD1	2.31	0.42
1:C:734:THR:HG23	1:C:767:LEU:HD12	2.02	0.42
1:A:66:HIS:HD2	1:A:68:ILE:CG2	2.32	0.42
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.38	0.42
1:B:428:ASP:OD1	1:B:428:ASP:N	2.49	0.42
1:B:431:GLY:HA2	1:B:515:PHE:HZ	1.85	0.42
1:B:471:GLU:N	1:B:471:GLU:CD	2.78	0.42
1:B:533:LEU:HD12	1:B:534:VAL:C	2.45	0.42
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.53	0.42
1:C:96:GLU:HB3	1:C:99:ASN:HA	2.01	0.42
1:C:368:LEU:H	1:C:368:LEU:CD1	2.33	0.42
1:C:498:GLN:HG2	1:C:499:PRO:HD2	2.02	0.42
1:C:662:CYS:SG	1:C:697:MET:HB2	2.57	0.42
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.87	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.38	0.42
1:A:1043:CYS:CA	1:A:1064:HIS:HE1	2.27	0.42
1:B:55:PHE:HB3	1:B:275:PHE:HE2	1.79	0.42
1:B:599:THR:CB	1:B:608:VAL:HG12	2.50	0.42
1:B:773:GLU:OE2	1:B:1019:ARG:HG3	2.19	0.42
1:B:1078:ALA:N	1:B:1102:TRP:HH2	2.18	0.42
1:C:718:PHE:HD2	1:C:1109:PHE:HE1	1.68	0.42
1:C:800:PHE:CD1	1:C:898:PHE:CE2	3.08	0.42
1:A:33:THR:CB	1:A:58:PHE:CZ	3.00	0.41
1:A:321:GLN:HA	1:A:322:PRO:HD3	1.95	0.41
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.35	0.41
1:B:528:LYS:HB3	1:B:528:LYS:NZ	2.34	0.41
1:B:708:SER:HB2	1:B:711:SER:CB	2.50	0.41
1:B:795:LYS:O	1:B:796:ASP:C	2.62	0.41
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.53	0.41
1:C:164:ASN:C	1:C:164:ASN:ND2	2.78	0.41
1:C:516:GLU:CG	1:C:519:HIS:CE1	2.97	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLY:H	1:B:235:ILE:HG23	1.85	0.41
1:C:37:TYR:CD1	1:C:37:TYR:N	2.87	0.41
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.85	0.41
1:C:105:ILE:HG12	1:C:118:LEU:HD13	1.96	0.41
1:C:117:LEU:C	1:C:117:LEU:CD2	2.93	0.41
1:C:138:ASP:N	1:C:139:PRO:HD3	2.35	0.41
1:C:317:ASN:CA	1:C:593:GLY:O	2.68	0.41
1:C:715:PRO:CA	1:C:1071:GLN:O	2.65	0.41
1:C:726:ILE:CD1	1:C:1061:VAL:HG22	2.49	0.41
1:A:55:PHE:CD1	1:A:275:PHE:HD2	2.38	0.41
1:A:119:ILE:HG13	1:A:128:ILE:HG12	2.01	0.41
1:A:290:ASP:O	1:A:297:SER:HB3	2.20	0.41
1:A:612:TYR:HB3	1:A:615:VAL:CG2	2.50	0.41
1:B:91:TYR:O	1:B:91:TYR:CD1	2.74	0.41
1:B:902:MET:CB	1:B:916:LEU:HD21	2.40	0.41
1:B:976:VAL:HG12	1:B:979:ASP:H	1.86	0.41
1:C:320:VAL:HG11	1:C:619:GLU:OE2	2.21	0.41
1:C:718:PHE:CZ	1:C:923:ILE:HD11	2.55	0.41
1:C:734:THR:HG21	1:C:1011:GLN:HE21	1.84	0.41
1:C:808:ASP:HA	1:C:809:PRO:HD3	1.95	0.41
1:C:931:ILE:HA	1:C:931:ILE:HD13	1.97	0.41
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.55	0.41
1:A:775:ASP:OD2	1:A:864:LEU:HD22	2.21	0.41
1:A:804:GLN:HE21	1:A:804:GLN:HB3	1.63	0.41
1:A:927:PHE:CD1	1:A:927:PHE:C	2.98	0.41
1:A:992:GLN:NE2	1:A:992:GLN:CA	2.81	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CG	2.55	0.41
1:B:417:LYS:O	1:B:421:TYR:HB2	2.21	0.41
1:B:541:PHE:CE1	1:B:587:ILE:CD1	2.90	0.41
1:B:825:LYS:NZ	1:B:945:LEU:HD12	2.35	0.41
1:C:55:PHE:C	1:C:270:LEU:HB3	2.45	0.41
1:C:349:SER:OG	1:C:451:TYR:HA	2.20	0.41
1:A:357:ARG:CD	1:B:230:PRO:HB2	2.50	0.41
1:A:805:ILE:HB	1:A:878:LEU:HD11	2.03	0.41
1:A:874:THR:HG21	1:A:1055:SER:HB3	2.01	0.41
1:B:212:LEU:CD1	1:B:214:ARG:N	2.83	0.41
1:B:961:THR:HG22	1:B:965:GLN:OE1	2.20	0.41
1:C:328:ARG:HD3	1:C:531:THR:O	2.21	0.41
1:C:555:SER:OG	1:C:585:LEU:HA	2.20	0.41
1:C:660:TYR:CB	1:C:695:TYR:CE2	3.00	0.41
1:A:230:PRO:HG2	1:C:357:ARG:NH1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.28	0.41
1:A:536:ASN:N	1:A:536:ASN:ND2	2.68	0.41
1:B:195:LYS:HE2	1:B:197:ILE:CG1	2.51	0.41
1:B:555:SER:HA	1:B:586:ASP:OD1	2.20	0.41
1:C:204:TYR:HD1	1:C:225:PRO:CB	2.31	0.41
1:C:241:LEU:CD1	1:C:241:LEU:N	2.84	0.41
1:C:532:ASN:N	1:C:532:ASN:HD22	2.17	0.41
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.53	0.41
1:A:37:TYR:N	1:A:37:TYR:CD1	2.88	0.41
1:A:43:PHE:CD1	1:A:43:PHE:C	2.99	0.41
1:A:864:LEU:O	1:A:864:LEU:HG	2.19	0.41
1:B:270:LEU:HD12	1:B:270:LEU:N	2.33	0.41
1:B:294:ASP:N	1:B:297:SER:HB2	2.33	0.41
1:B:555:SER:CB	1:B:586:ASP:OD1	2.69	0.41
1:C:15:CYS:SG	1:C:16:VAL:N	2.93	0.41
1:C:164:ASN:ND2	1:C:164:ASN:O	2.54	0.41
1:C:423:TYR:HE2	1:C:425:LEU:HD21	1.82	0.41
1:C:720:ILE:HD12	1:C:1049:LEU:CD1	2.50	0.41
1:A:17:ASN:O	1:A:255:SER:HA	2.21	0.41
1:A:458:LYS:HD3	1:A:473:TYR:CE2	2.56	0.41
1:A:569:ILE:HG23	1:B:47:VAL:CG1	2.51	0.41
1:A:1079:PRO:HA	1:B:900:MET:HE3	2.03	0.41
1:B:88:ASP:OD1	1:B:88:ASP:N	2.54	0.41
1:B:805:ILE:CG2	1:B:878:LEU:CD1	2.99	0.41
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.47	0.41
1:C:736:VAL:HG23	1:C:857:GLY:C	2.45	0.41
1:A:203:ILE:CG2	1:A:227:VAL:HG22	2.51	0.41
1:A:328:ARG:NH2	1:A:533:LEU:CA	2.84	0.41
1:A:328:ARG:NH2	1:A:533:LEU:N	2.69	0.41
1:A:335:LEU:HD12	1:A:335:LEU:O	2.21	0.41
1:A:368:LEU:HD11	2:E:1:NAG:H81	2.03	0.41
1:A:483:VAL:HG13	1:A:485:GLY:H	1.86	0.41
1:A:962:LEU:HA	1:A:965:GLN:CG	2.50	0.41
1:A:1023:ASN:O	1:A:1027:THR:OG1	2.24	0.41
1:B:133:PHE:CE1	1:B:163:ALA:HB2	2.55	0.41
1:B:212:LEU:C	1:B:212:LEU:CD1	2.93	0.41
1:B:354:ASN:O	1:B:398:ASP:HA	2.20	0.41
1:B:382:VAL:N	1:C:984:LEU:HD13	2.36	0.41
1:B:501:ASN:HB3	1:B:505:TYR:HB2	2.01	0.41
1:B:542:ASN:N	1:B:547:THR:HG23	2.34	0.41
1:B:583:GLU:OE1	1:B:583:GLU:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:PHE:HD2	1:B:927:PHE:CE2	2.37	0.41
1:B:805:ILE:CD1	1:B:1052:PHE:CD2	3.03	0.41
1:C:117:LEU:HD21	1:C:119:ILE:CD1	2.51	0.41
1:C:210:ILE:CD1	1:C:210:ILE:N	2.83	0.41
1:C:781:VAL:HG13	1:C:1026:ALA:HA	2.02	0.41
1:C:786:LYS:N	1:C:786:LYS:HE3	2.35	0.41
1:A:56:LEU:HD11	1:A:60:SER:HB3	2.03	0.41
1:A:295:PRO:HB2	1:A:608:VAL:HG21	2.03	0.41
1:A:405:ASP:OD1	1:A:405:ASP:N	2.54	0.41
1:A:612:TYR:HB2	1:A:615:VAL:CG2	2.51	0.41
1:A:1048:HIS:O	1:A:1048:HIS:CG	2.73	0.41
1:B:360:ASN:OD1	1:B:523:THR:HG23	2.15	0.41
1:B:794:ILE:HG22	1:B:796:ASP:H	1.86	0.41
1:C:353:TRP:CE3	1:C:423:TYR:HB2	2.16	0.41
1:C:738:CYS:HB3	1:C:1004:LEU:HD11	2.03	0.41
1:C:807:PRO:CG	1:C:875:SER:HB2	2.50	0.41
1:A:231:ILE:HG22	1:A:233:ILE:N	2.29	0.40
1:A:241:LEU:HD12	1:A:242:LEU:H	1.80	0.40
1:A:349:SER:O	1:A:352:ALA:O	2.39	0.40
1:A:697:MET:HE1	1:B:865:LEU:HD23	2.03	0.40
1:A:864:LEU:HD11	1:C:665:PRO:CB	2.52	0.40
1:A:884:SER:O	1:A:884:SER:OG	2.39	0.40
1:A:1007:TYR:CE1	1:A:1011:GLN:OE1	2.74	0.40
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	2.03	0.40
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.02	0.40
1:B:537:LYS:O	1:B:551:VAL:HA	2.20	0.40
1:B:773:GLU:O	1:B:777:ASN:CG	2.63	0.40
1:B:1081:ILE:CD1	1:B:1133:VAL:HG23	2.50	0.40
1:C:380:TYR:HE2	1:C:412:PRO:HD2	1.76	0.40
1:C:792:PRO:O	1:C:793:PRO:C	2.65	0.40
1:A:752:LEU:HD12	1:A:993:ILE:HG21	2.02	0.40
1:A:826:VAL:HG22	1:A:945:LEU:CD1	2.33	0.40
1:A:890:ALA:CB	1:C:1046:GLY:HA3	2.51	0.40
1:A:1032:CYS:HB3	1:A:1051:SER:CB	2.48	0.40
1:A:1078:ALA:CB	1:A:1102:TRP:HH2	2.34	0.40
1:B:56:LEU:HD12	1:B:57:PRO:HD3	1.98	0.40
1:B:131:CYS:SG	1:B:166:CYS:HB3	2.61	0.40
1:B:1095:PHE:HZ	1:B:1120:THR:CG2	2.25	0.40
1:C:337:PRO:HB2	1:C:340:GLU:HG2	2.03	0.40
1:C:365:TYR:HD2	1:C:387:LEU:HD13	1.86	0.40
1:C:497:PHE:CE1	1:C:507:PRO:HA	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:LYS:HA	1:C:812:PRO:HD3	1.93	0.40
1:A:211:ASN:HD22	1:A:211:ASN:H	1.68	0.40
1:A:280:ASN:HD22	1:A:286:THR:CG2	2.34	0.40
1:A:453:TYR:OH	1:A:493:GLN:HG3	2.20	0.40
1:A:864:LEU:HD11	1:C:665:PRO:HB2	2.02	0.40
1:A:998:THR:O	1:A:1002:GLN:HG2	2.21	0.40
1:A:1090:PRO:HG3	1:A:1093:GLY:O	2.21	0.40
1:A:1115:ILE:H	1:A:1115:ILE:HG13	1.64	0.40
1:B:985:ASP:O	1:B:989:ALA:CA	2.66	0.40
1:B:1116:THR:CG2	1:B:1140:PRO:HD3	2.43	0.40
1:B:1121:PHE:C	1:B:1121:PHE:CD1	2.99	0.40
1:C:353:TRP:CH2	1:C:423:TYR:CA	3.04	0.40
1:C:453:TYR:CZ	1:C:493:GLN:NE2	2.90	0.40
1:C:480:CYS:SG	1:C:483:VAL:HG12	2.61	0.40
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.36	0.40
1:A:280:ASN:HD22	1:A:286:THR:HG21	1.84	0.40
1:A:791:THR:HA	1:A:792:PRO:HD2	1.88	0.40
1:A:962:LEU:HD22	1:A:1007:TYR:CB	2.52	0.40
1:A:1029:MET:N	1:A:1062:PHE:CE2	2.89	0.40
1:B:125:ASN:CG	1:B:172:SER:O	2.65	0.40
1:B:198:ASP:OD1	1:B:200:TYR:CE2	2.74	0.40
1:B:456:PHE:CD1	1:B:490:PHE:O	2.75	0.40
1:B:729:VAL:H	1:B:1059:GLY:HA2	1.86	0.40
1:B:773:GLU:O	1:B:777:ASN:CB	2.69	0.40
1:C:17:ASN:O	1:C:255:SER:HA	2.22	0.40
1:C:119:ILE:HG23	1:C:120:VAL:N	2.35	0.40
1:C:273:ARG:HB2	1:C:275:PHE:CE1	2.56	0.40
1:A:115:GLN:CD	1:A:130:VAL:CG1	2.95	0.40
1:A:353:TRP:CD1	1:A:353:TRP:N	2.89	0.40
1:A:612:TYR:HB3	1:A:615:VAL:HG22	2.02	0.40
1:B:277:LEU:HD12	1:B:288:ALA:CB	2.51	0.40
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.04	0.40
1:B:471:GLU:HA	1:B:471:GLU:OE1	2.22	0.40
1:B:541:PHE:HZ	1:B:587:ILE:HD13	1.73	0.40
1:B:577:ARG:CA	1:B:584:ILE:HA	2.51	0.40
1:B:884:SER:O	1:B:887:THR:OG1	2.27	0.40
1:B:1115:ILE:O	1:B:1138:TYR:CD1	2.72	0.40
1:C:320:VAL:HG21	1:C:619:GLU:OE2	2.21	0.40
1:C:337:PRO:HB2	1:C:340:GLU:CG	2.52	0.40
1:C:492:LEU:HD22	1:C:492:LEU:N	2.36	0.40
1:C:528:LYS:N	1:C:528:LYS:HD2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:773:GLU:HA	1:C:776:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1070/1270 (84%)	1017 (95%)	46 (4%)	7 (1%)	18	55
1	B	1071/1270 (84%)	1025 (96%)	38 (4%)	8 (1%)	18	55
1	C	1066/1270 (84%)	1020 (96%)	44 (4%)	2 (0%)	43	77
All	All	3207/3810 (84%)	3062 (96%)	128 (4%)	17 (0%)	26	62

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	A	620	VAL
1	B	332	ILE
1	B	371	SER
1	B	857	GLY
1	B	946	GLY
1	A	502	GLY
1	A	619	GLU
1	A	1053	PRO
1	A	337	PRO
1	B	728	PRO
1	B	1140	PRO
1	C	529	LYS
1	C	665	PRO
1	A	637	SER
1	B	1112	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	337	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	938/1102 (85%)	878 (94%)	60 (6%)	16	38
1	B	937/1102 (85%)	866 (92%)	71 (8%)	12	33
1	C	929/1102 (84%)	849 (91%)	80 (9%)	10	30
All	All	2804/3306 (85%)	2593 (92%)	211 (8%)	14	33

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	62	VAL
1	A	66	HIS
1	A	88	ASP
1	A	117	LEU
1	A	136	CYS
1	A	211	ASN
1	A	227	VAL
1	A	229	LEU
1	A	235	ILE
1	A	237	ARG
1	A	240	THR
1	A	241	LEU
1	A	266	TYR
1	A	301	CYS
1	A	332	ILE
1	A	353	TRP
1	A	445	VAL
1	A	452	LEU
1	A	501	ASN
1	A	515	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	LEU
1	A	536	ASN
1	A	552	LEU
1	A	567	ARG
1	A	595	VAL
1	A	599	THR
1	A	602	THR
1	A	611	LEU
1	A	650	LEU
1	A	654	GLU
1	A	693	ILE
1	A	695	TYR
1	A	696	THR
1	A	697	MET
1	A	705	VAL
1	A	709	ASN
1	A	738	CYS
1	A	804	GLN
1	A	827	THR
1	A	954	GLN
1	A	961	THR
1	A	962	LEU
1	A	964	LYS
1	A	981	LEU
1	A	991	VAL
1	A	992	GLN
1	A	1004	LEU
1	A	1019	ARG
1	A	1031	GLU
1	A	1032	CYS
1	A	1048	HIS
1	A	1065	VAL
1	A	1068	VAL
1	A	1072	GLU
1	A	1103	PHE
1	A	1106	GLN
1	A	1115	ILE
1	A	1121	PHE
1	A	1127	ASP
1	B	86	PHE
1	B	88	ASP
1	B	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	119	ILE
1	B	122	ASN
1	B	141	LEU
1	B	193	VAL
1	B	216	LEU
1	B	218	GLN
1	B	220	PHE
1	B	226	LEU
1	B	234	ASN
1	B	265	TYR
1	B	270	LEU
1	B	277	LEU
1	B	289	VAL
1	B	301	CYS
1	B	302	THR
1	B	312	ILE
1	B	318	PHE
1	B	329	PHE
1	B	332	ILE
1	B	365	TYR
1	B	466	ARG
1	B	471	GLU
1	B	518	LEU
1	B	524	VAL
1	B	528	LYS
1	B	533	LEU
1	B	546	LEU
1	B	547	THR
1	B	553	THR
1	B	557	LYS
1	B	559	PHE
1	B	584	ILE
1	B	613	GLN
1	B	620	VAL
1	B	644	GLN
1	B	651	ILE
1	B	658	ASN
1	B	699	LEU
1	B	712	ILE
1	B	737	ASP
1	B	740	MET
1	B	747	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	784	GLN
1	B	786	LYS
1	B	787	GLN
1	B	817	PHE
1	B	818	ILE
1	B	826	VAL
1	B	888	PHE
1	B	896	ILE
1	B	919	ASN
1	B	933	LYS
1	B	950	ASP
1	B	1004	LEU
1	B	1009	THR
1	B	1011	GLN
1	B	1050	MET
1	B	1065	VAL
1	B	1072	GLU
1	B	1104	VAL
1	B	1116	THR
1	B	1125	ASN
1	B	1128	VAL
1	B	1130	ILE
1	B	1132	ILE
1	B	1134	ASN
1	B	1141	LEU
1	B	1145	LEU
1	C	43	PHE
1	C	48	LEU
1	C	51	THR
1	C	54	LEU
1	C	55	PHE
1	C	87	ASN
1	C	96	GLU
1	C	99	ASN
1	C	105	ILE
1	C	119	ILE
1	C	195	LYS
1	C	210	ILE
1	C	212	LEU
1	C	213	VAL
1	C	216	LEU
1	C	220	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	223	LEU
1	C	226	LEU
1	C	229	LEU
1	C	233	ILE
1	C	266	TYR
1	C	270	LEU
1	C	282	ASN
1	C	314	GLN
1	C	334	ASN
1	C	340	GLU
1	C	345	THR
1	C	365	TYR
1	C	367	VAL
1	C	368	LEU
1	C	388	ASN
1	C	393	THR
1	C	406	GLU
1	C	409	GLN
1	C	445	VAL
1	C	461	LEU
1	C	483	VAL
1	C	517	LEU
1	C	518	LEU
1	C	528	LYS
1	C	529	LYS
1	C	531	THR
1	C	555	SER
1	C	582	LEU
1	C	585	LEU
1	C	588	THR
1	C	611	LEU
1	C	613	GLN
1	C	618	THR
1	C	655	HIS
1	C	658	ASN
1	C	660	TYR
1	C	671	CYS
1	C	692	ILE
1	C	699	LEU
1	C	786	LYS
1	C	822	LEU
1	C	826	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	856	ASN
1	C	861	LEU
1	C	881	THR
1	C	895	GLN
1	C	896	ILE
1	C	921	LYS
1	C	931	ILE
1	C	934	ILE
1	C	951	VAL
1	C	969	ASN
1	C	981	LEU
1	C	984	LEU
1	C	993	ILE
1	C	1005	GLN
1	C	1065	VAL
1	C	1083	HIS
1	C	1092	GLU
1	C	1098	ASN
1	C	1101	HIS
1	C	1129	VAL
1	C	1135	ASN
1	C	1139	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	66	HIS
1	A	87	ASN
1	A	99	ASN
1	A	211	ASN
1	A	317	ASN
1	A	321	GLN
1	A	334	ASN
1	A	360	ASN
1	A	394	ASN
1	A	409	GLN
1	A	501	ASN
1	A	536	ASN
1	A	580	GLN
1	A	613	GLN
1	A	675	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	690	GLN
1	A	751	ASN
1	A	755	GLN
1	A	764	ASN
1	A	774	GLN
1	A	779	GLN
1	A	901	GLN
1	A	954	GLN
1	A	965	GLN
1	A	978	ASN
1	A	1002	GLN
1	A	1011	GLN
1	A	1108	ASN
1	A	1113	GLN
1	A	1142	GLN
1	B	49	HIS
1	B	99	ASN
1	B	122	ASN
1	B	165	ASN
1	B	207	HIS
1	B	211	ASN
1	B	218	GLN
1	B	245	HIS
1	B	314	GLN
1	B	317	ASN
1	B	334	ASN
1	B	422	ASN
1	B	448	ASN
1	B	501	ASN
1	B	544	ASN
1	B	563	GLN
1	B	564	GLN
1	B	606	ASN
1	B	607	GLN
1	B	784	GLN
1	B	824	ASN
1	B	913	GLN
1	B	920	GLN
1	B	955	ASN
1	B	965	GLN
1	B	1002	GLN
1	B	1011	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1036	GLN
1	B	1058	HIS
1	B	1101	HIS
1	B	1119	ASN
1	B	1142	GLN
1	C	17	ASN
1	C	99	ASN
1	C	164	ASN
1	C	185	ASN
1	C	314	GLN
1	C	321	GLN
1	C	360	ASN
1	C	388	ASN
1	C	394	ASN
1	C	409	GLN
1	C	414	GLN
1	C	474	GLN
1	C	493	GLN
1	C	532	ASN
1	C	544	ASN
1	C	607	GLN
1	C	644	GLN
1	C	655	HIS
1	C	690	GLN
1	C	751	ASN
1	C	762	GLN
1	C	779	GLN
1	C	824	ASN
1	C	901	GLN
1	C	992	GLN
1	C	1036	GLN
1	C	1048	HIS
1	C	1064	HIS
1	C	1083	HIS
1	C	1088	HIS
1	C	1125	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

20 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	0.80	0	17,19,21	3.07	7 (41%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	1.12	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.79	0	17,19,21	2.96	6 (35%)
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	1.12	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.81	0	17,19,21	2.98	7 (41%)
2	NAG	F	2	2	14,14,15	0.65	0	17,19,21	1.13	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.76	0	17,19,21	3.02	6 (35%)
2	NAG	G	2	2	14,14,15	0.65	0	17,19,21	1.14	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	3.02	7 (41%)
2	NAG	H	2	2	14,14,15	0.63	0	17,19,21	1.13	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.82	0	17,19,21	2.97	7 (41%)
2	NAG	I	2	2	14,14,15	0.63	0	17,19,21	1.12	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.79	0	17,19,21	3.04	7 (41%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	1.10	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.78	0	17,19,21	3.11	7 (41%)
2	NAG	K	2	2	14,14,15	0.67	0	17,19,21	1.11	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.80	0	17,19,21	2.99	7 (41%)
2	NAG	L	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.81	0	17,19,21	3.18	6 (35%)
2	NAG	M	2	2	14,14,15	0.69	0	17,19,21	1.15	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O7-C7	-2.02	1.18	1.23

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C8-C7-N2	7.72	128.91	116.12
2	K	1	NAG	C8-C7-N2	7.63	128.78	116.12
2	H	1	NAG	C8-C7-N2	7.58	128.69	116.12
2	J	1	NAG	C8-C7-N2	7.56	128.66	116.12
2	D	1	NAG	C8-C7-N2	7.49	128.54	116.12
2	M	1	NAG	C8-C7-N2	7.36	128.32	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C8-C7-N2	7.35	128.31	116.12
2	G	1	NAG	C8-C7-N2	7.27	128.17	116.12
2	I	1	NAG	C8-C7-N2	7.26	128.16	116.12
2	M	1	NAG	C2-N2-C7	7.22	132.58	122.90
2	F	1	NAG	C8-C7-N2	7.22	128.09	116.12
2	K	1	NAG	C2-N2-C7	6.99	132.27	122.90
2	D	1	NAG	C2-N2-C7	6.77	131.98	122.90
2	H	1	NAG	C2-N2-C7	6.62	131.78	122.90
2	L	1	NAG	C2-N2-C7	6.58	131.72	122.90
2	J	1	NAG	C2-N2-C7	6.55	131.68	122.90
2	F	1	NAG	C2-N2-C7	6.53	131.65	122.90
2	G	1	NAG	C2-N2-C7	6.47	131.57	122.90
2	E	1	NAG	C2-N2-C7	6.38	131.45	122.90
2	I	1	NAG	C2-N2-C7	6.35	131.40	122.90
2	M	1	NAG	O7-C7-N2	-5.24	112.71	121.98
2	J	1	NAG	O7-C7-N2	-5.16	112.86	121.98
2	K	1	NAG	O7-C7-N2	-5.05	113.06	121.98
2	E	1	NAG	O7-C7-N2	-5.04	113.08	121.98
2	D	1	NAG	O7-C7-N2	-4.99	113.16	121.98
2	G	1	NAG	O7-C7-N2	-4.94	113.25	121.98
2	L	1	NAG	O7-C7-N2	-4.77	113.56	121.98
2	I	1	NAG	O7-C7-N2	-4.56	113.92	121.98
2	F	1	NAG	O7-C7-N2	-4.55	113.93	121.98
2	H	1	NAG	O7-C7-N2	-4.54	113.96	121.98
2	G	1	NAG	C4-C3-C2	-3.69	105.61	111.02
2	M	1	NAG	C1-O5-C5	-3.66	107.29	112.19
2	I	1	NAG	C1-O5-C5	-3.46	107.54	112.19
2	L	1	NAG	C1-O5-C5	-3.27	107.80	112.19
2	F	1	NAG	C1-O5-C5	-3.22	107.87	112.19
2	F	1	NAG	C4-C3-C2	-3.07	106.52	111.02
2	I	1	NAG	C4-C3-C2	-2.99	106.64	111.02
2	M	1	NAG	C4-C3-C2	-2.98	106.65	111.02
2	K	1	NAG	C1-O5-C5	-2.94	108.25	112.19
2	G	1	NAG	C1-O5-C5	-2.93	108.26	112.19
2	D	1	NAG	C4-C3-C2	-2.92	106.74	111.02
2	H	1	NAG	C1-O5-C5	-2.88	108.33	112.19
2	K	1	NAG	C1-C2-N2	-2.87	105.91	110.43
2	M	1	NAG	C1-C2-N2	-2.87	105.92	110.43
2	D	1	NAG	C1-C2-N2	-2.86	105.92	110.43
2	K	1	NAG	C4-C3-C2	-2.67	107.11	111.02
2	H	1	NAG	O7-C7-C8	-2.66	117.32	122.05
2	H	1	NAG	C1-C2-N2	-2.64	106.27	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	NAG	C2-N2-C7	-2.64	119.37	122.90
2	D	1	NAG	C1-O5-C5	-2.63	108.66	112.19
2	G	1	NAG	C1-C2-N2	-2.58	106.36	110.43
2	E	2	NAG	C2-N2-C7	-2.56	119.47	122.90
2	F	2	NAG	C1-C2-N2	-2.54	106.42	110.43
2	L	1	NAG	C4-C3-C2	-2.54	107.29	111.02
2	H	1	NAG	C4-C3-C2	-2.54	107.30	111.02
2	D	2	NAG	C2-N2-C7	-2.53	119.52	122.90
2	D	2	NAG	C1-C2-N2	-2.52	106.47	110.43
2	J	2	NAG	C1-C2-N2	-2.52	106.47	110.43
2	L	2	NAG	C2-N2-C7	-2.51	119.53	122.90
2	G	2	NAG	C2-N2-C7	-2.51	119.54	122.90
2	I	2	NAG	C1-C2-N2	-2.50	106.50	110.43
2	J	1	NAG	C1-C2-N2	-2.50	106.50	110.43
2	H	2	NAG	C1-C2-N2	-2.49	106.51	110.43
2	G	2	NAG	C1-C2-N2	-2.48	106.52	110.43
2	L	2	NAG	C1-C2-N2	-2.47	106.53	110.43
2	J	1	NAG	C1-O5-C5	-2.47	108.88	112.19
2	J	2	NAG	C2-N2-C7	-2.46	119.60	122.90
2	K	2	NAG	C2-N2-C7	-2.46	119.61	122.90
2	H	2	NAG	C2-N2-C7	-2.45	119.61	122.90
2	K	2	NAG	C1-C2-N2	-2.43	106.60	110.43
2	M	2	NAG	C1-C2-N2	-2.43	106.60	110.43
2	J	1	NAG	C4-C3-C2	-2.43	107.46	111.02
2	F	1	NAG	C1-C2-N2	-2.40	106.64	110.43
2	E	2	NAG	C1-C2-N2	-2.40	106.65	110.43
2	F	2	NAG	C2-N2-C7	-2.39	119.70	122.90
2	I	2	NAG	C2-N2-C7	-2.38	119.71	122.90
2	L	1	NAG	C1-C2-N2	-2.37	106.71	110.43
2	E	1	NAG	C4-C3-C2	-2.34	107.58	111.02
2	I	1	NAG	O7-C7-C8	-2.33	117.91	122.05
2	F	1	NAG	O7-C7-C8	-2.29	117.97	122.05
2	E	1	NAG	O7-C7-C8	-2.28	118.00	122.05
2	E	1	NAG	C1-C2-N2	-2.27	106.86	110.43
2	L	1	NAG	O7-C7-C8	-2.20	118.13	122.05
2	K	1	NAG	O7-C7-C8	-2.20	118.14	122.05
2	D	1	NAG	O7-C7-C8	-2.13	118.27	122.05
2	I	1	NAG	C1-C2-N2	-2.12	107.09	110.43
2	J	1	NAG	O7-C7-C8	-2.02	118.45	122.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1
2	H	1	NAG	C1
2	I	1	NAG	C1
2	L	1	NAG	C1

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	M	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

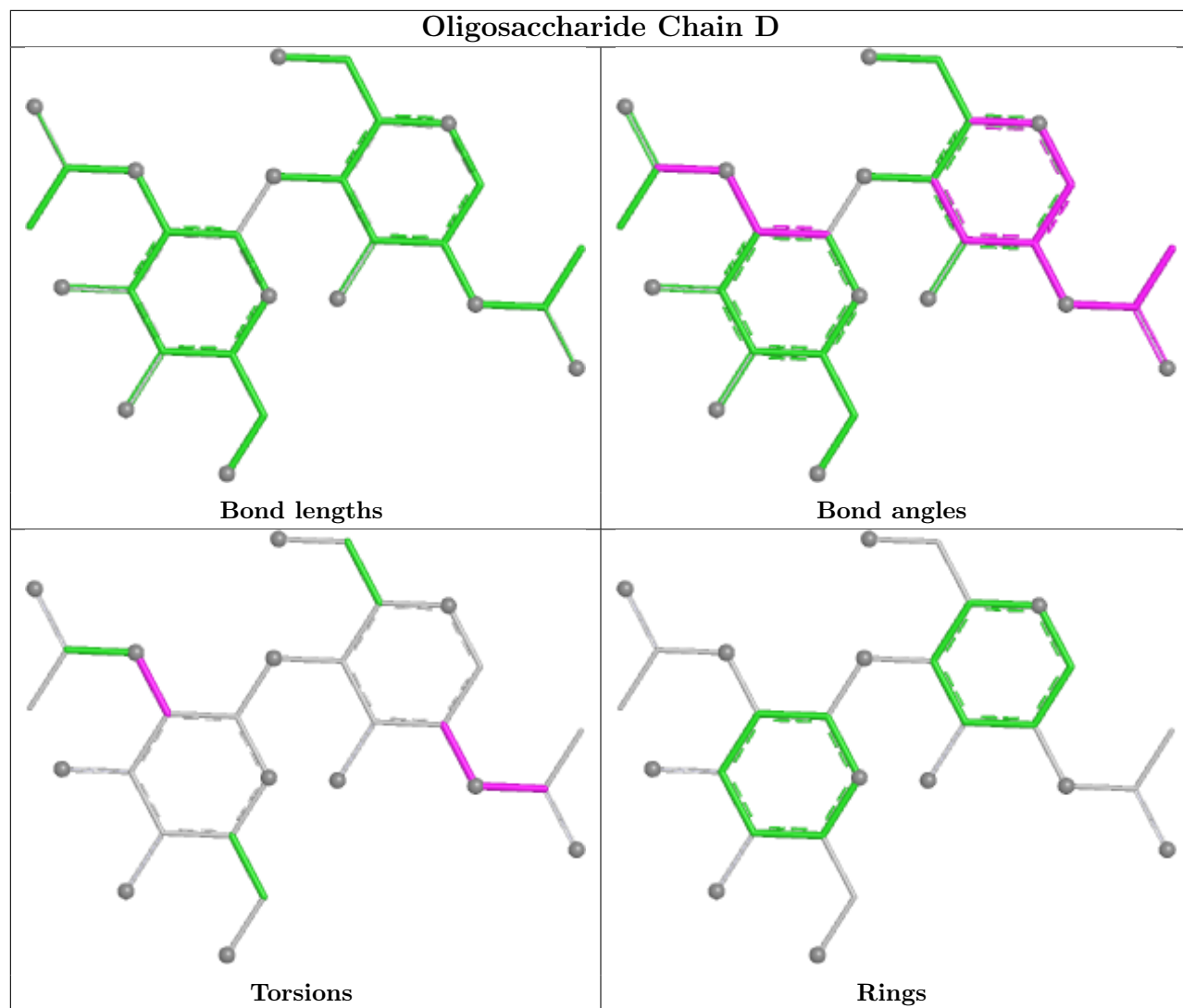
Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	M	2	NAG	C3-C2-N2-C7

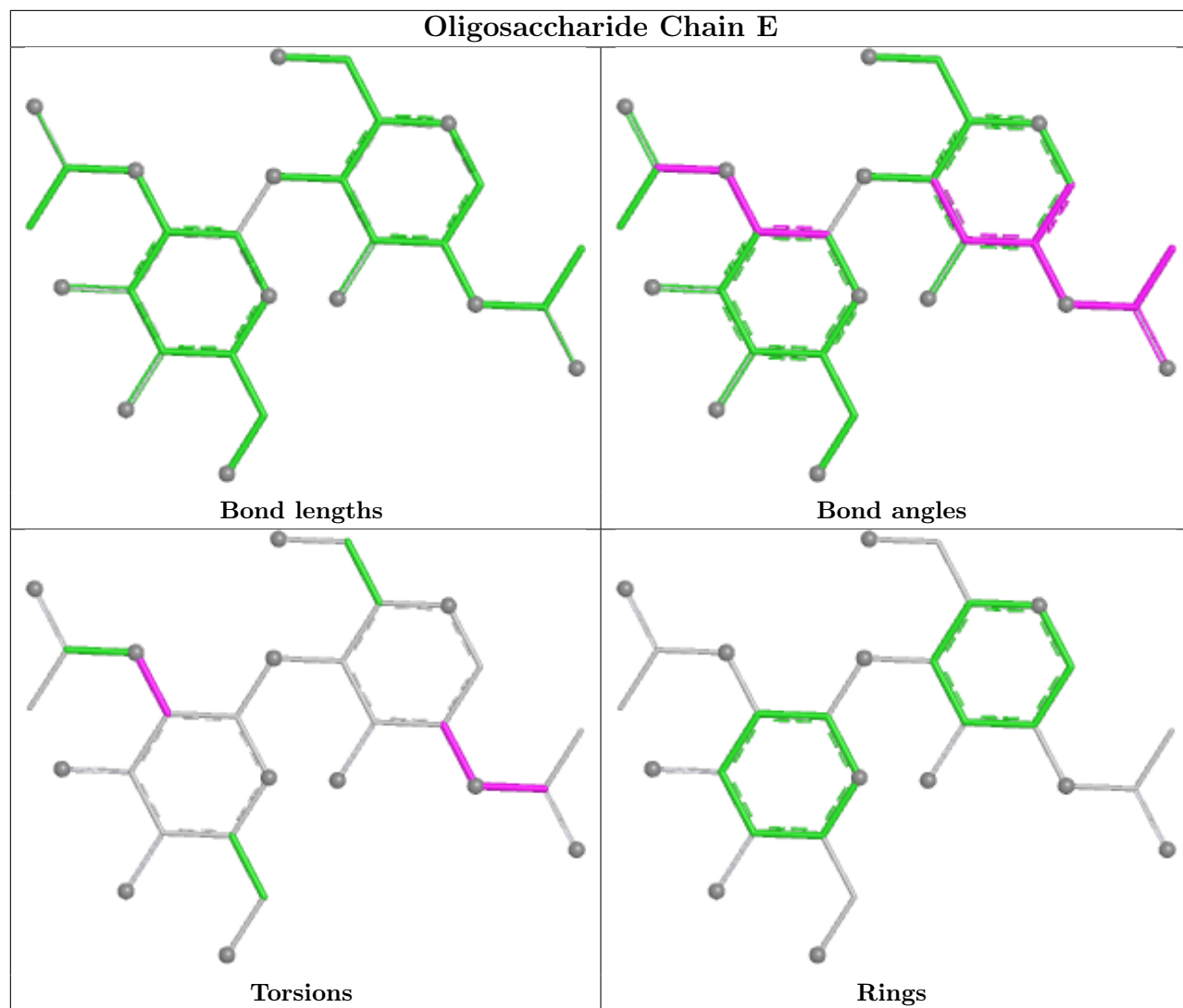
There are no ring outliers.

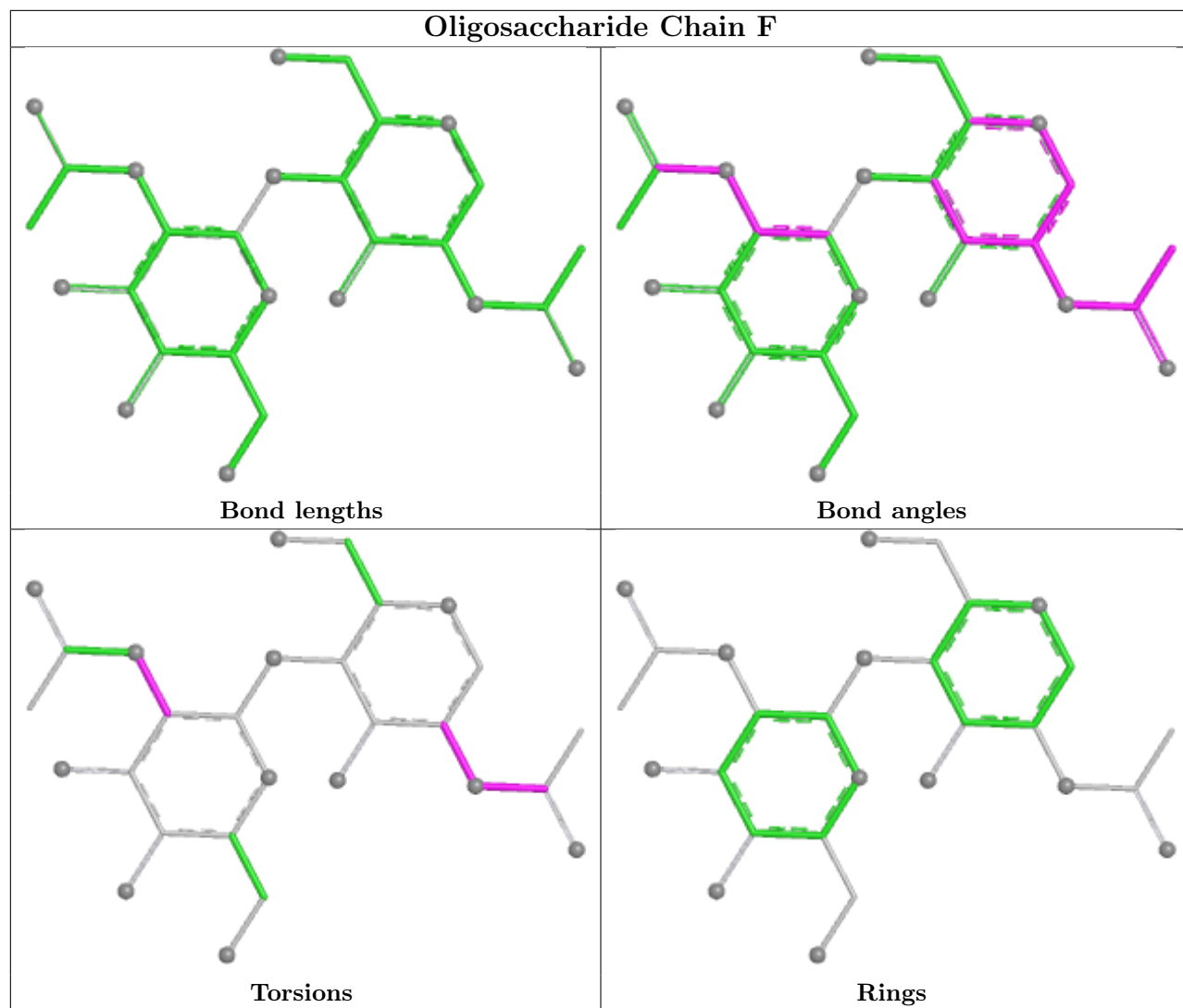
3 monomers are involved in 3 short contacts:

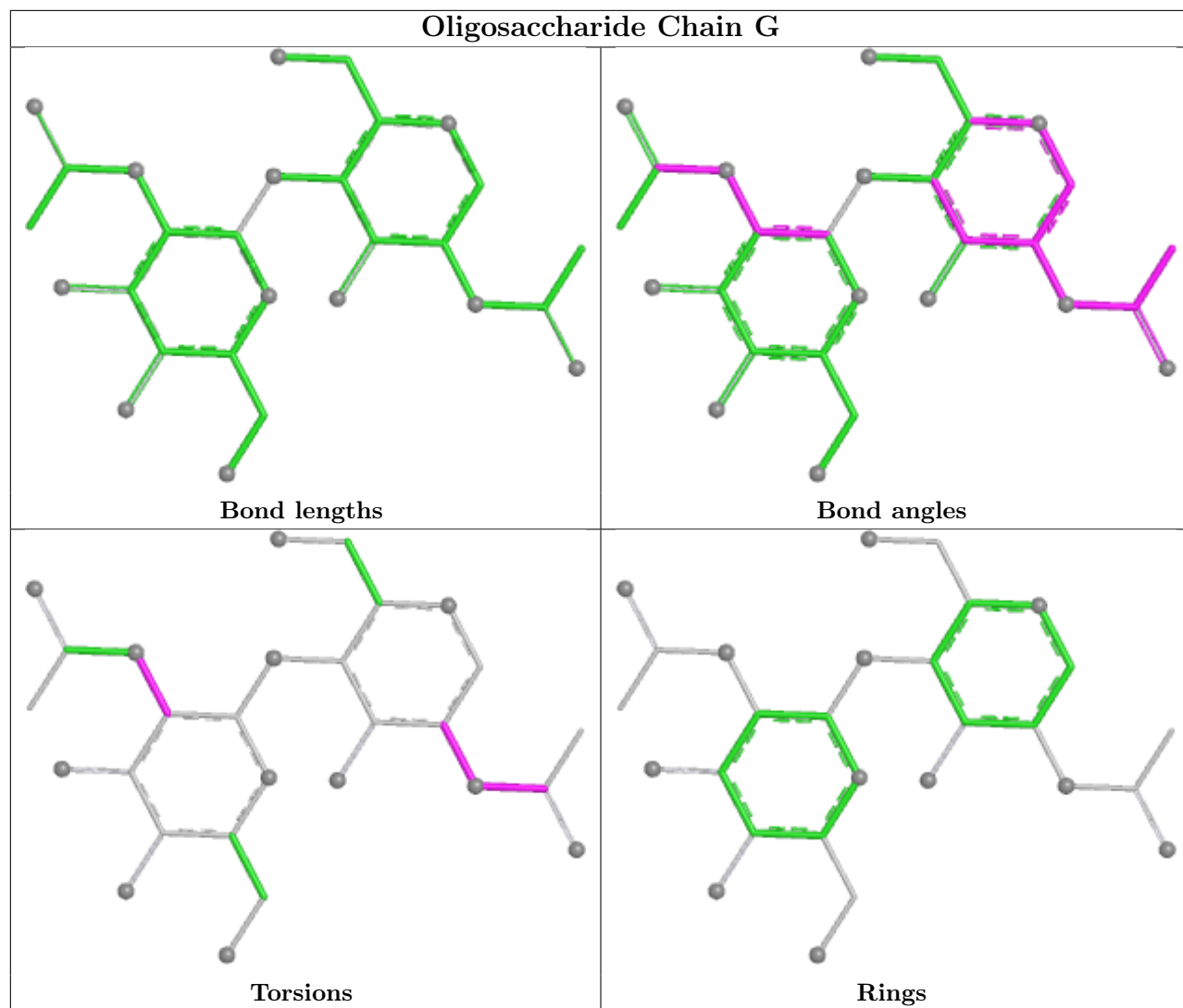
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	E	1	NAG	1	0
2	F	1	NAG	1	0

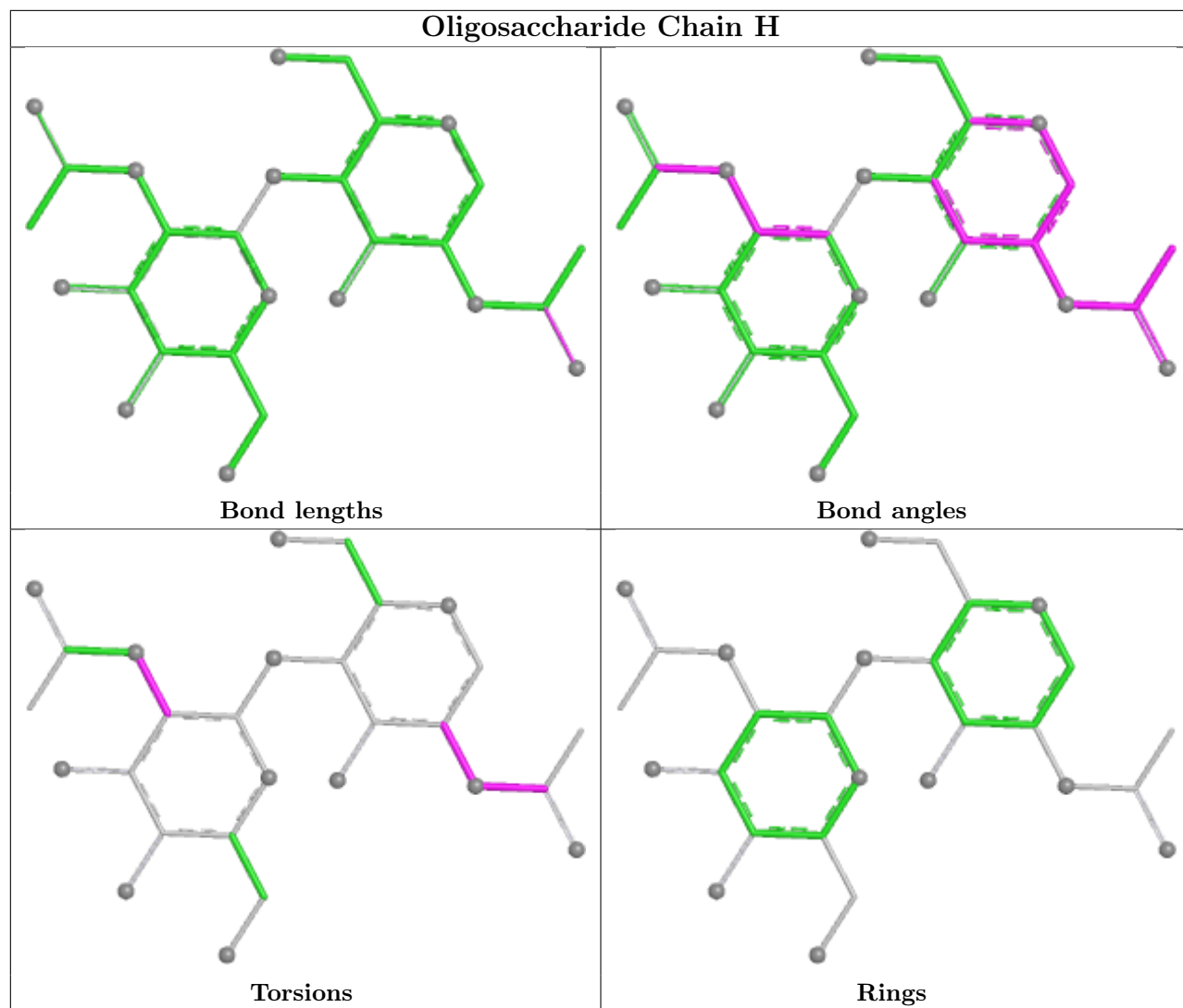
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

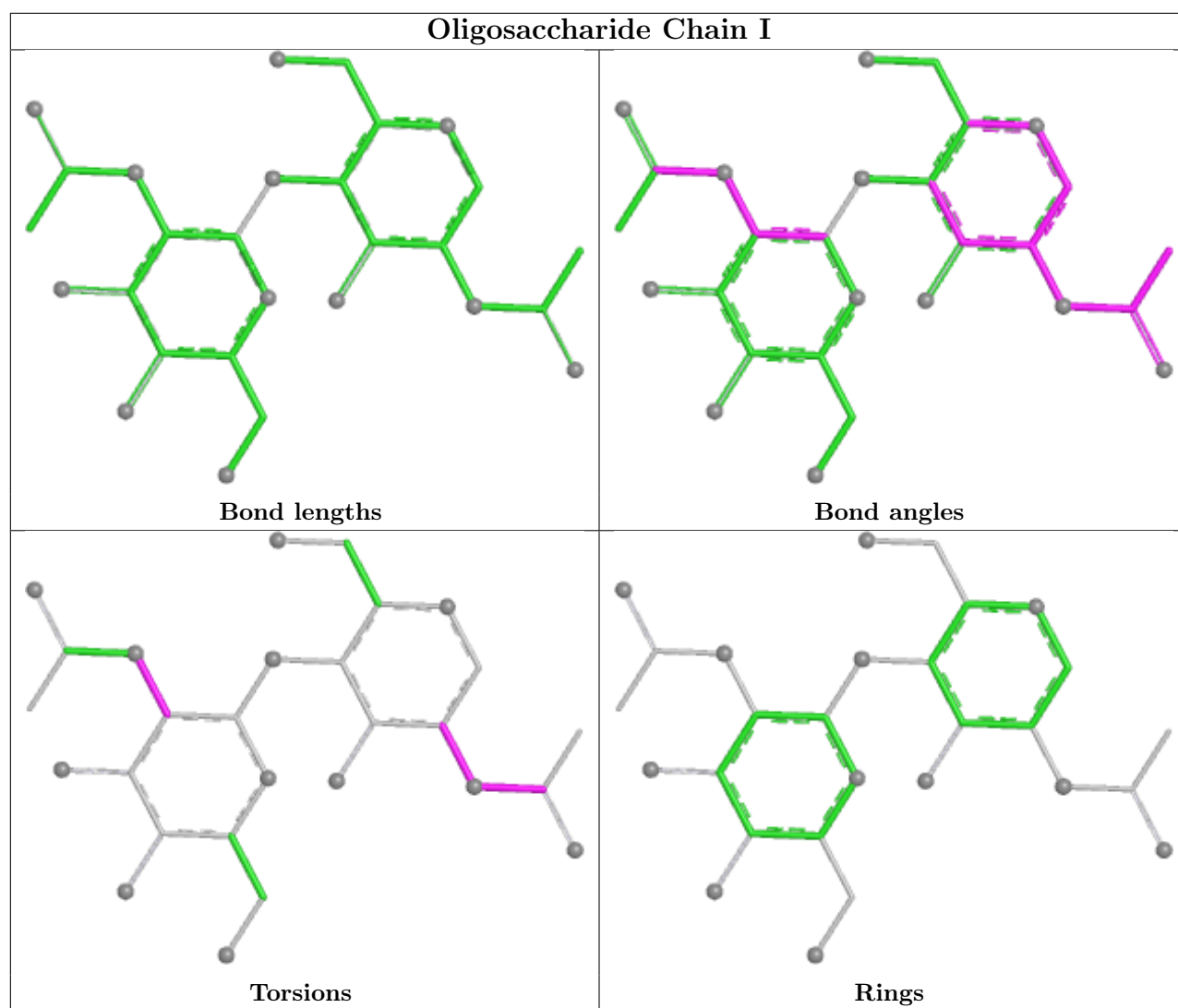


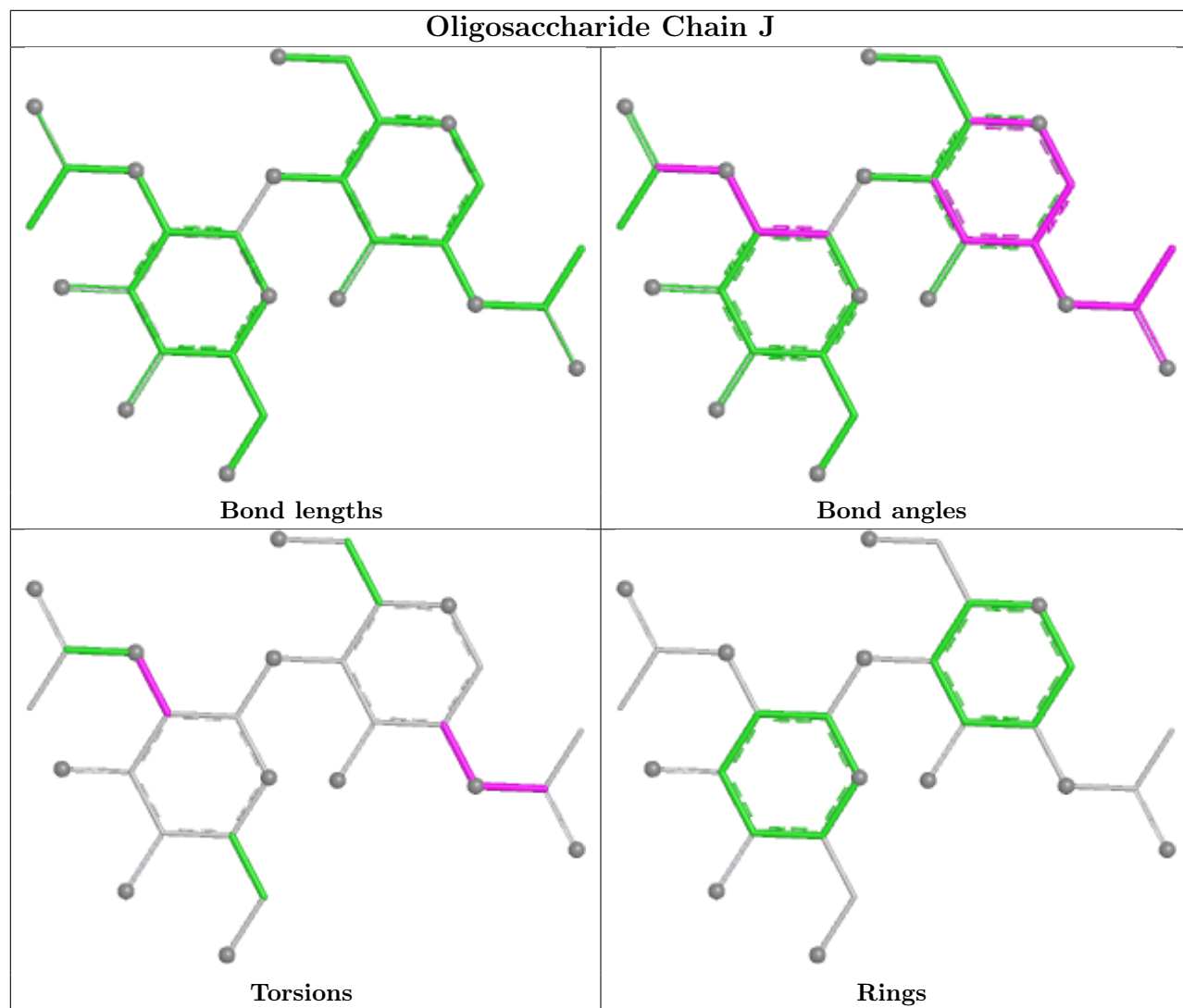


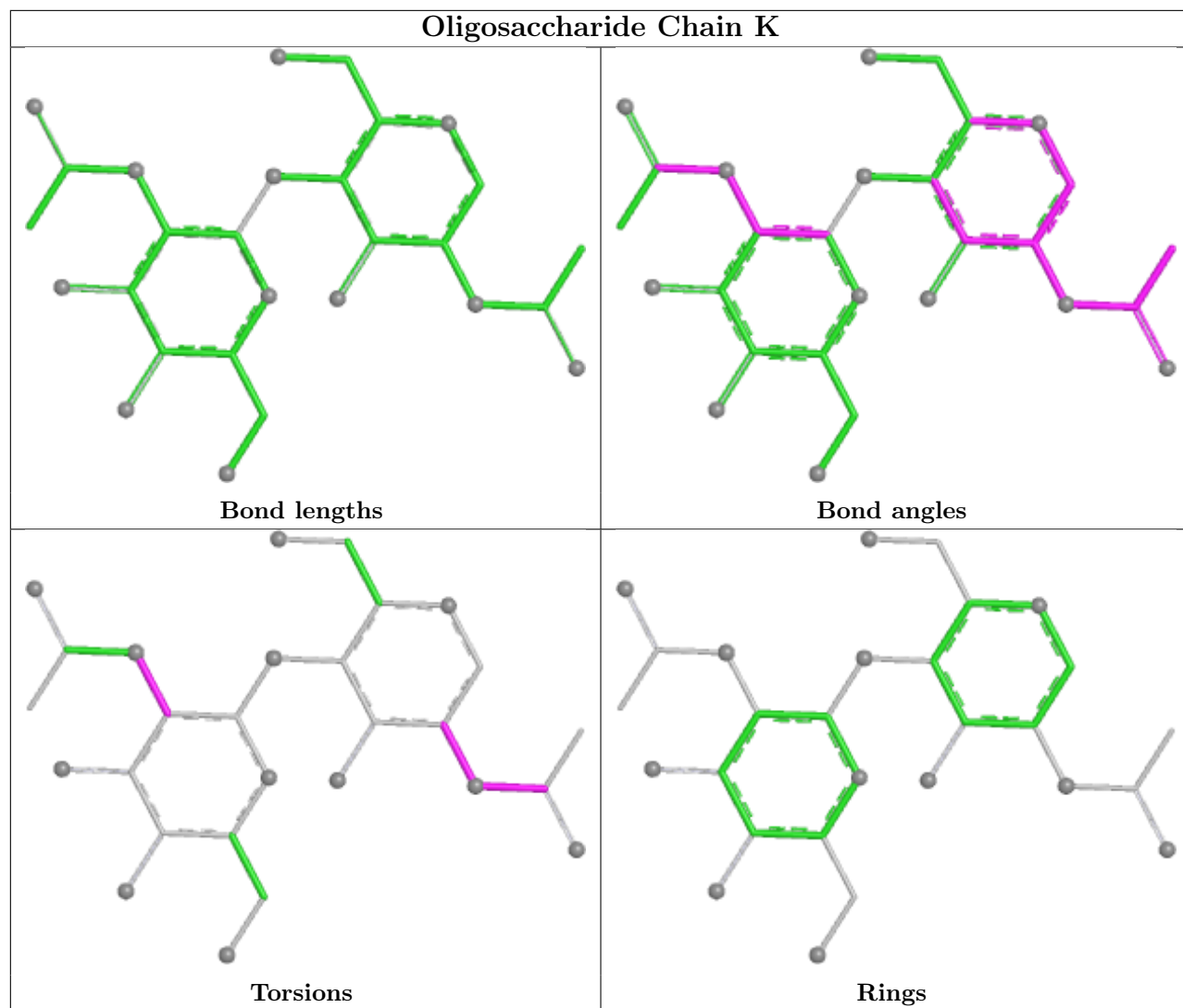


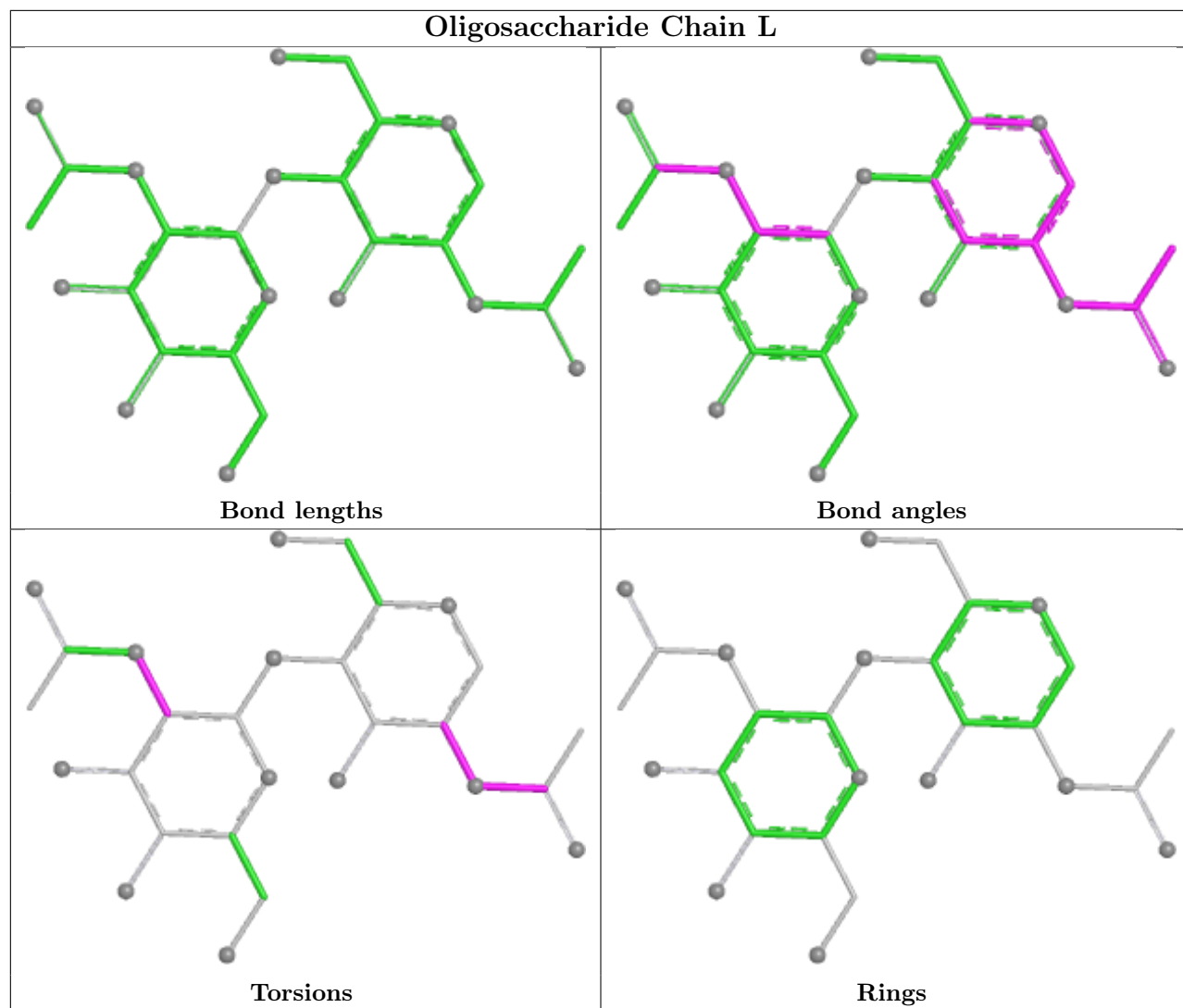


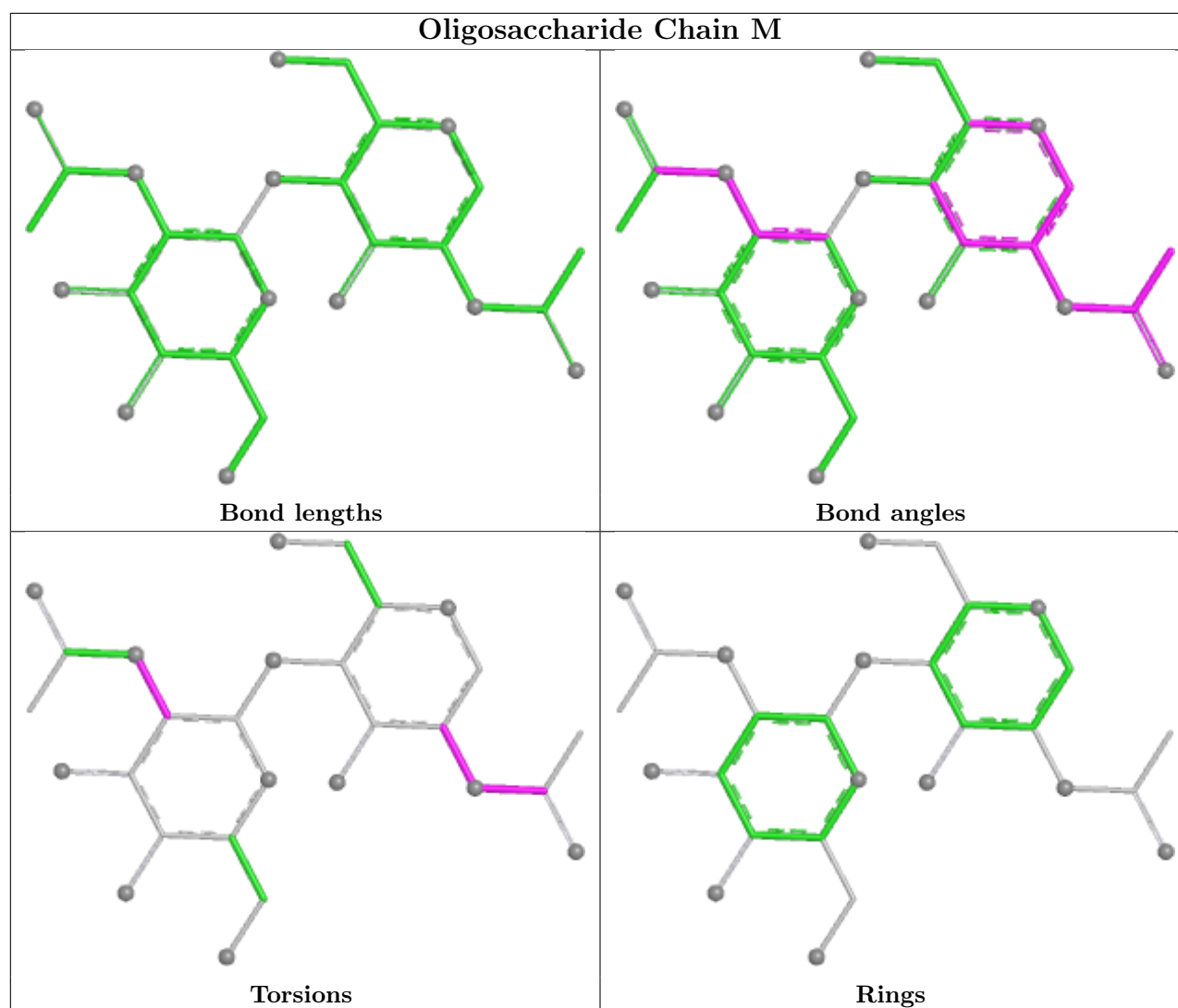












5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1301	1	14,14,15	0.33	0	17,19,21	0.63	0
5	XIO	C	1307	4	97,101,101	2.37	32 (32%)	119,143,143	1.17	13 (10%)
3	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1309	1	14,14,15	0.95	1 (7%)	17,19,21	1.77	5 (29%)
3	NAG	A	1306	1	14,14,15	0.42	0	17,19,21	2.51	5 (29%)
3	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	1.43	3 (17%)
3	NAG	B	1306	1	14,14,15	0.58	0	17,19,21	1.10	2 (11%)
3	NAG	C	1303	1	14,14,15	2.02	2 (14%)	17,19,21	3.26	4 (23%)
3	NAG	C	1305	1	14,14,15	0.46	0	17,19,21	0.74	0
3	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	1.31	2 (11%)
3	NAG	B	1307	1	14,14,15	0.57	0	17,19,21	1.31	2 (11%)
3	NAG	B	1301	1	14,14,15	0.60	0	17,19,21	1.40	2 (11%)
3	NAG	A	1309	1	14,14,15	0.46	0	17,19,21	1.16	1 (5%)
3	NAG	B	1308	1	14,14,15	0.46	0	17,19,21	2.02	5 (29%)
3	NAG	C	1302	1	14,14,15	0.46	0	17,19,21	1.50	3 (17%)
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	B	1303	1	14,14,15	0.63	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	1.59	3 (17%)
3	NAG	A	1305	1	14,14,15	0.37	0	17,19,21	0.83	1 (5%)
3	NAG	A	1308	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	1305	1	14,14,15	0.54	0	17,19,21	1.42	3 (17%)
3	NAG	B	1304	1	14,14,15	0.48	0	17,19,21	0.99	0
3	NAG	C	1306	1	14,14,15	0.47	0	17,19,21	1.59	3 (17%)
3	NAG	A	1307	1	14,14,15	0.66	1 (7%)	17,19,21	1.69	2 (11%)
3	NAG	B	1302	1	14,14,15	0.89	0	17,19,21	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
5	XIO	C	1307	4	-	26/79/85/85	0/9/9/9
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1307	XIO	C08-N09	7.05	1.49	1.34
5	C	1307	XIO	C43-N44	6.86	1.48	1.34
5	C	1307	XIO	C02-N71	6.53	1.47	1.34
5	C	1307	XIO	C37-N36	6.53	1.45	1.34
3	C	1303	NAG	C1-C2	6.48	1.61	1.52
5	C	1307	XIO	C48-S49	5.83	1.83	1.75
5	C	1307	XIO	C13-S14	5.30	1.82	1.75
5	C	1307	XIO	C75-S76	5.03	1.82	1.75
5	C	1307	XIO	C06-C05	4.52	1.58	1.54
5	C	1307	XIO	C15-S14	4.38	1.83	1.78
5	C	1307	XIO	C50-S49	3.90	1.83	1.78
5	C	1307	XIO	C73-C74	3.83	1.55	1.50
5	C	1307	XIO	C77-S76	3.31	1.82	1.78
5	C	1307	XIO	C88-C87	-3.28	1.37	1.41
5	C	1307	XIO	C11-C12	3.21	1.54	1.50
5	C	1307	XIO	C07-C08	3.20	1.57	1.51
5	C	1307	XIO	O94-C93	3.08	1.40	1.30
5	C	1307	XIO	O32-C31	3.07	1.40	1.30
5	C	1307	XIO	C46-C47	3.01	1.54	1.50
5	C	1307	XIO	O83-N81	-3.00	1.17	1.22
5	C	1307	XIO	O67-C66	2.99	1.40	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1309	NAG	C1-C2	2.79	1.56	1.52
5	C	1307	XIO	C61-C60	-2.76	1.38	1.41
5	C	1307	XIO	C03-C02	2.75	1.56	1.51
5	C	1307	XIO	O56-N54	-2.67	1.18	1.22
5	C	1307	XIO	O21-N19	-2.59	1.18	1.22
5	C	1307	XIO	O40-C37	-2.53	1.18	1.23
5	C	1307	XIO	C26-C25	-2.47	1.38	1.41
5	C	1307	XIO	O01-C02	-2.25	1.18	1.23
5	C	1307	XIO	C26-C12	-2.17	1.40	1.44
5	C	1307	XIO	C13-N24	-2.15	1.32	1.37
5	C	1307	XIO	C48-N59	-2.15	1.32	1.37
3	C	1303	NAG	O5-C5	2.14	1.47	1.43
5	C	1307	XIO	C42-C43	2.10	1.55	1.51
5	C	1307	XIO	O35-C08	-2.08	1.19	1.23
3	A	1307	NAG	C1-C2	2.08	1.55	1.52
3	B	1303	NAG	C1-C2	2.02	1.55	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1303	NAG	C1-O5-C5	11.65	127.80	112.19
3	A	1306	NAG	C2-N2-C7	6.40	131.47	122.90
3	A	1306	NAG	C8-C7-N2	5.87	125.85	116.12
3	B	1308	NAG	C8-C7-N2	5.24	124.81	116.12
3	A	1307	NAG	O5-C1-C2	-4.74	103.95	111.29
5	C	1307	XIO	C05-N36-C37	-4.33	119.97	126.42
3	B	1302	NAG	O5-C1-C2	-4.29	104.65	111.29
3	B	1309	NAG	O5-C1-C2	-4.27	104.68	111.29
3	C	1304	NAG	C8-C7-N2	4.22	123.11	116.12
3	B	1305	NAG	O5-C1-C2	-4.18	104.82	111.29
3	C	1306	NAG	C8-C7-N2	4.14	122.99	116.12
3	B	1301	NAG	O5-C1-C2	-3.94	105.19	111.29
3	B	1309	NAG	C1-O5-C5	3.93	117.45	112.19
3	C	1303	NAG	C2-N2-C7	3.92	128.16	122.90
3	B	1308	NAG	C2-N2-C7	3.75	127.92	122.90
3	C	1302	NAG	C8-C7-N2	3.67	122.20	116.12
3	B	1307	NAG	C2-N2-C7	3.65	127.79	122.90
3	C	1301	NAG	C8-C7-N2	3.63	122.14	116.12
3	A	1304	NAG	O5-C1-C2	-3.52	105.85	111.29
3	A	1309	NAG	O5-C1-C2	-3.45	105.96	111.29
3	C	1306	NAG	C2-N2-C7	3.36	127.40	122.90
3	B	1308	NAG	C1-C2-N2	-3.35	105.15	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1307	NAG	C1-C2-N2	3.32	115.66	110.43
5	C	1307	XIO	S49-C48-N59	3.14	126.04	121.93
3	C	1302	NAG	C2-N2-C7	3.12	127.08	122.90
3	B	1303	NAG	C1-O5-C5	3.06	116.28	112.19
3	A	1306	NAG	O7-C7-N2	-3.03	116.62	121.98
5	C	1307	XIO	S14-C13-N24	3.02	125.89	121.93
5	C	1307	XIO	S76-C75-N86	2.98	125.84	121.93
3	C	1303	NAG	C3-C4-C5	2.97	115.62	110.23
3	C	1304	NAG	C2-N2-C7	2.91	126.80	122.90
3	C	1301	NAG	C2-N2-C7	2.90	126.78	122.90
3	B	1308	NAG	O7-C7-N2	-2.85	116.95	121.98
3	B	1301	NAG	O5-C5-C6	2.76	113.04	107.66
3	A	1306	NAG	C1-O5-C5	2.73	115.85	112.19
5	C	1307	XIO	C42-C41-C05	-2.71	112.28	115.44
5	C	1307	XIO	C03-C04-C05	-2.70	112.29	115.44
5	C	1307	XIO	C07-C06-C05	-2.62	112.38	115.44
3	A	1305	NAG	O5-C1-C2	-2.55	107.35	111.29
3	A	1306	NAG	O7-C7-C8	-2.54	117.52	122.05
3	C	1302	NAG	O7-C7-N2	-2.54	117.50	121.98
3	C	1306	NAG	O7-C7-N2	-2.48	117.59	121.98
3	B	1307	NAG	O7-C7-N2	2.45	126.32	121.98
3	B	1306	NAG	C2-N2-C7	-2.39	119.69	122.90
5	C	1307	XIO	C07-C08-N09	2.34	119.98	115.86
5	C	1307	XIO	C42-C43-N44	2.32	119.95	115.86
5	C	1307	XIO	C03-C02-N71	2.30	119.92	115.86
3	A	1304	NAG	C2-N2-C7	2.27	125.95	122.90
5	C	1307	XIO	C30-C25-C26	-2.24	120.02	122.19
5	C	1307	XIO	C65-C60-C61	-2.24	120.02	122.19
3	C	1303	NAG	C1-C2-N2	-2.23	106.91	110.43
3	B	1309	NAG	C2-N2-C7	2.22	125.88	122.90
3	B	1308	NAG	O7-C7-C8	-2.20	118.13	122.05
3	B	1309	NAG	C1-C2-N2	2.18	113.86	110.43
3	B	1305	NAG	C1-O5-C5	2.18	115.10	112.19
3	C	1304	NAG	O7-C7-N2	-2.14	118.20	121.98
3	B	1306	NAG	C1-O5-C5	2.13	115.03	112.19
3	C	1301	NAG	O7-C7-N2	-2.12	118.24	121.98
5	C	1307	XIO	C92-C87-C88	-2.10	120.15	122.19
3	B	1309	NAG	C4-C3-C2	-2.06	108.00	111.02
3	B	1305	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1304	NAG	C3-C2-N2-C7
3	A	1306	NAG	C1-C2-N2-C7
5	C	1307	XIO	C31-C10-C11-C12
5	C	1307	XIO	C06-C05-N36-C37
5	C	1307	XIO	C41-C05-N36-C37
5	C	1307	XIO	C04-C05-N36-C37
5	C	1307	XIO	C52-C53-N54-O56
5	C	1307	XIO	C57-C53-N54-O56
5	C	1307	XIO	C72-C73-C74-C88
5	C	1307	XIO	C72-C73-C74-C75
5	C	1307	XIO	C31-C10-N09-C08
5	C	1307	XIO	C73-C72-N71-C02
3	B	1308	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
5	C	1307	XIO	C03-C02-N71-C72
3	B	1308	NAG	O5-C5-C6-O6
5	C	1307	XIO	O70-C43-N44-C45
5	C	1307	XIO	O01-C02-N71-C72
5	C	1307	XIO	N09-C10-C11-C12
3	A	1306	NAG	C8-C7-N2-C2
3	A	1306	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	C	1306	NAG	C8-C7-N2-C2
3	C	1306	NAG	O7-C7-N2-C2
3	B	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1302	NAG	O5-C5-C6-O6
5	C	1307	XIO	N71-C72-C93-O96
5	C	1307	XIO	N71-C72-C93-O94
3	B	1301	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
5	C	1307	XIO	C42-C43-N44-C45
3	B	1302	NAG	O5-C5-C6-O6
5	C	1307	XIO	N44-C45-C46-C47
3	A	1309	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	B	1309	NAG	C3-C2-N2-C7
3	C	1305	NAG	C3-C2-N2-C7
3	C	1304	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
5	C	1307	XIO	C66-C45-C46-C47
5	C	1307	XIO	C47-C48-S49-C50
5	C	1307	XIO	N09-C10-C31-O34
3	B	1307	NAG	C4-C5-C6-O6
5	C	1307	XIO	C73-C72-C93-O94
3	A	1306	NAG	C4-C5-C6-O6
5	C	1307	XIO	N09-C10-C31-O32
5	C	1307	XIO	C73-C72-C93-O96
3	B	1304	NAG	C4-C5-C6-O6
5	C	1307	XIO	N36-C05-C06-C07
5	C	1307	XIO	N44-C45-C66-O69

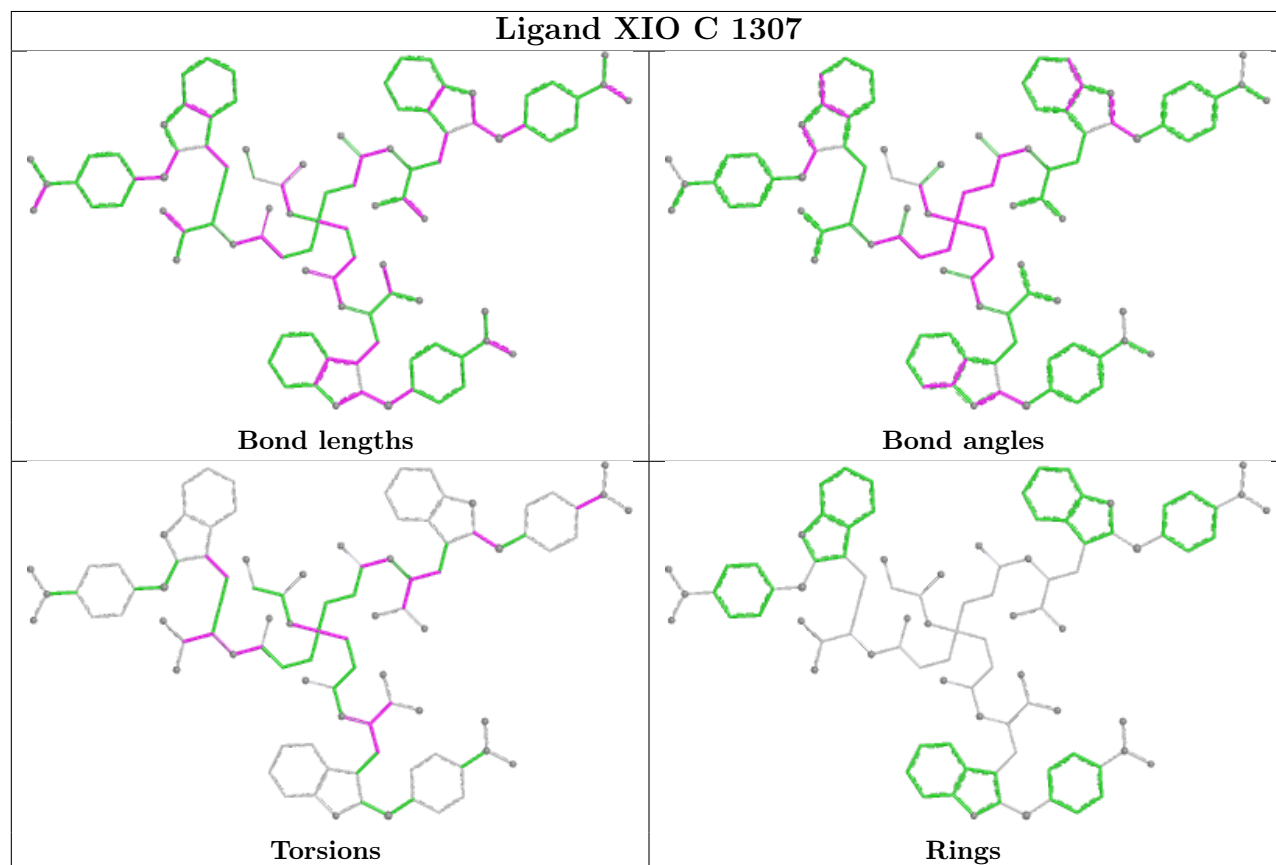
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1306	NAG	1	0
3	C	1305	NAG	1	0
3	B	1308	NAG	2	0
3	A	1308	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

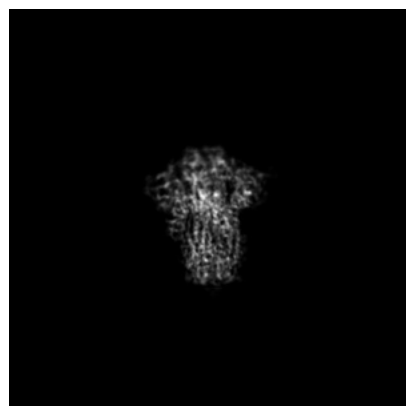
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17578. These allow visual inspection of the internal detail of the map and identification of artifacts.

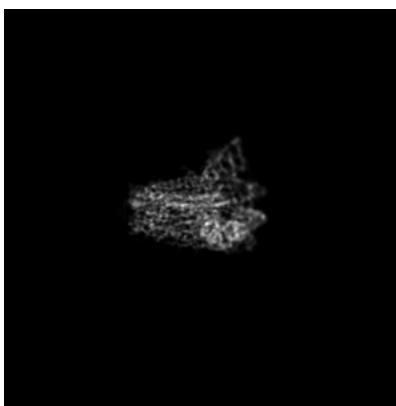
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

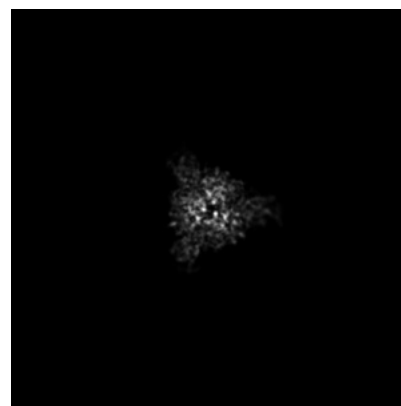
6.1.1 Primary map



X

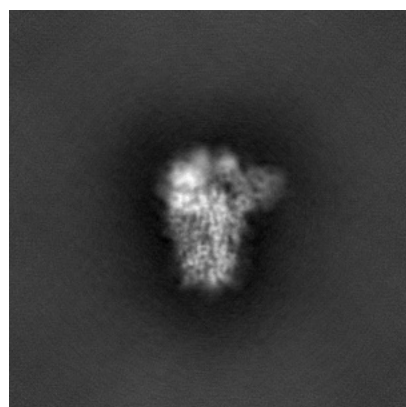


Y

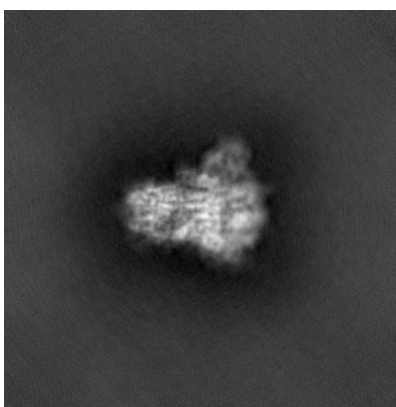


Z

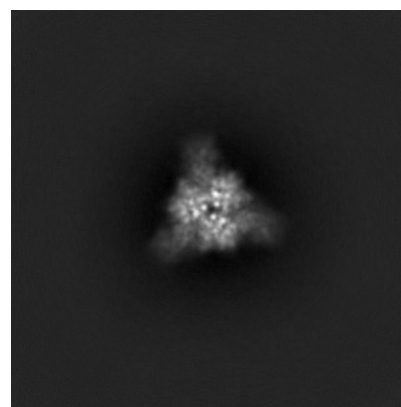
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

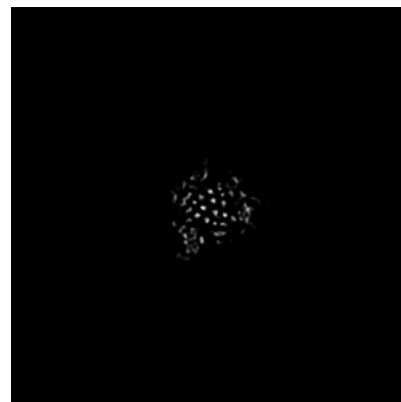
6.2.1 Primary map



X Index: 246

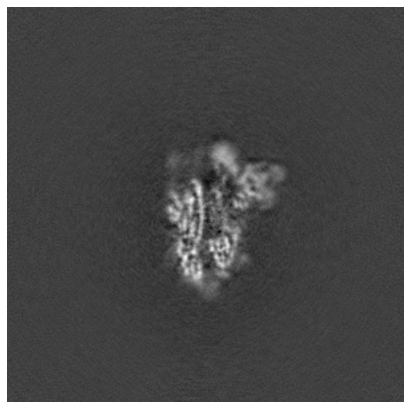


Y Index: 246

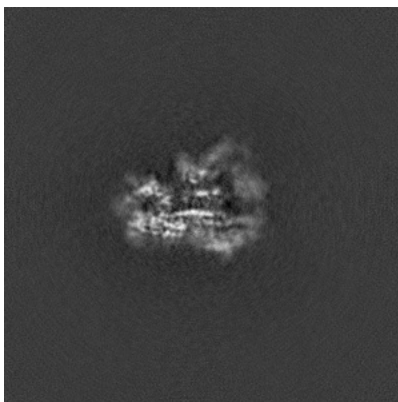


Z Index: 246

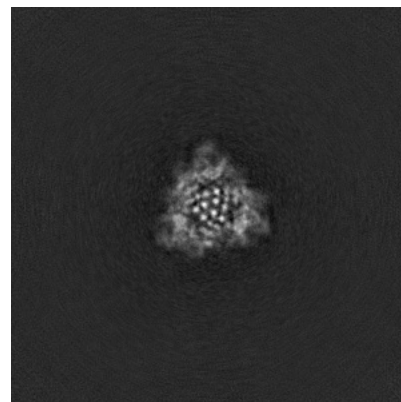
6.2.2 Raw map



X Index: 246



Y Index: 246



Z Index: 246

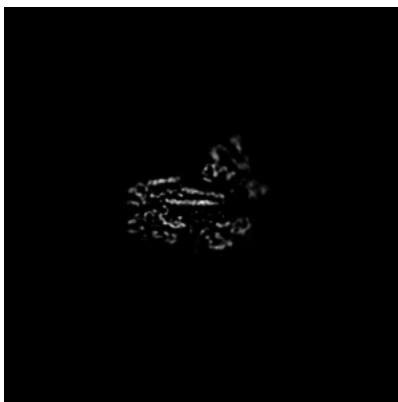
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 251

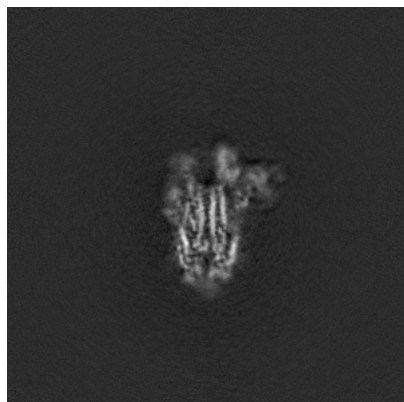


Y Index: 239

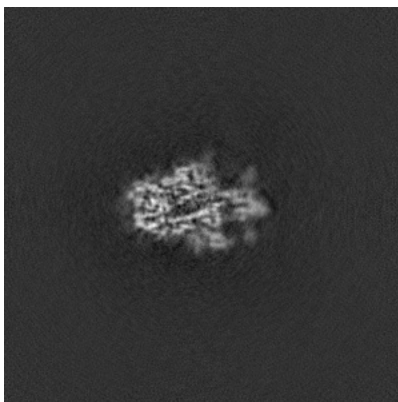


Z Index: 248

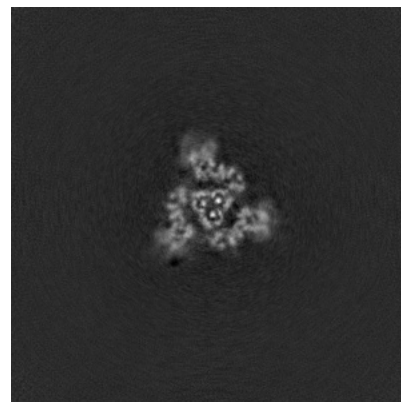
6.3.2 Raw map



X Index: 251



Y Index: 260

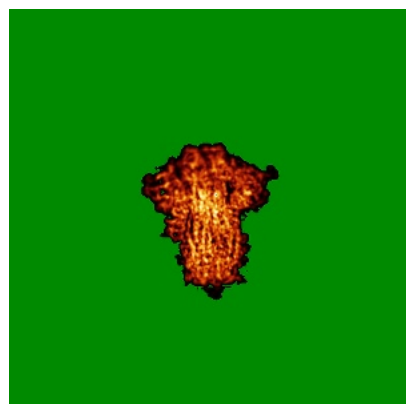


Z Index: 262

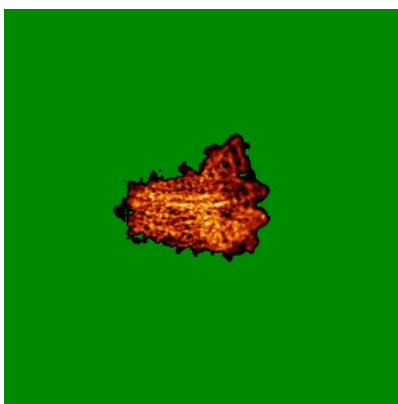
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

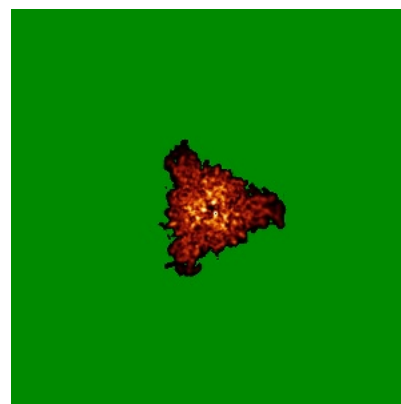
6.4.1 Primary map



X

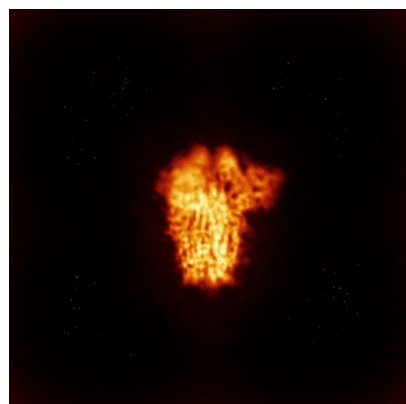


Y

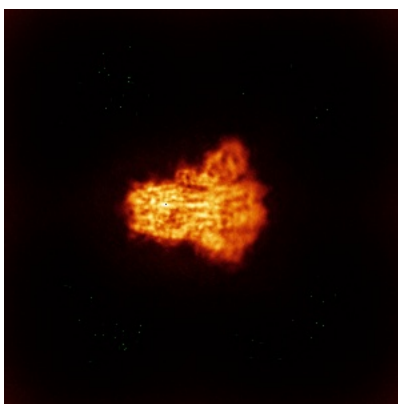


Z

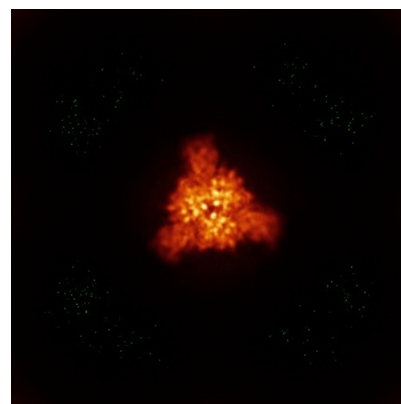
6.4.2 Raw map



X



Y

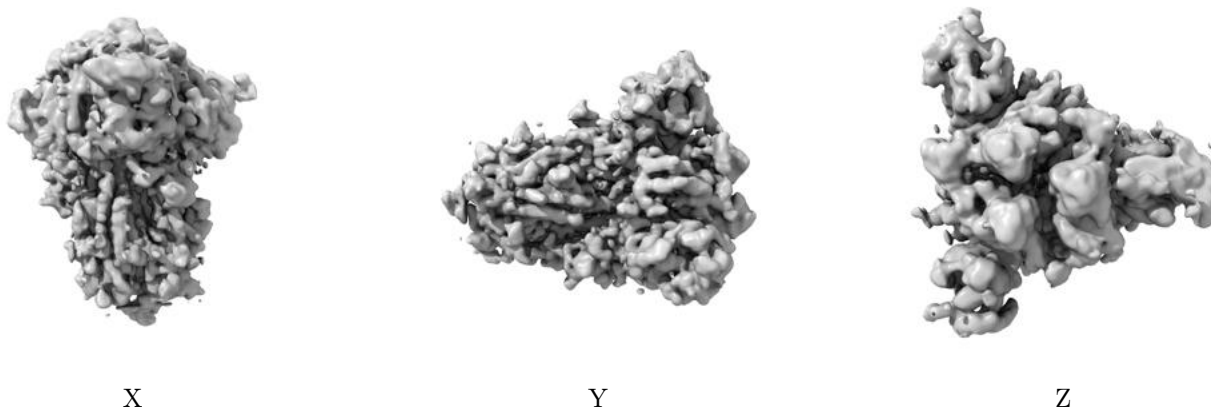


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

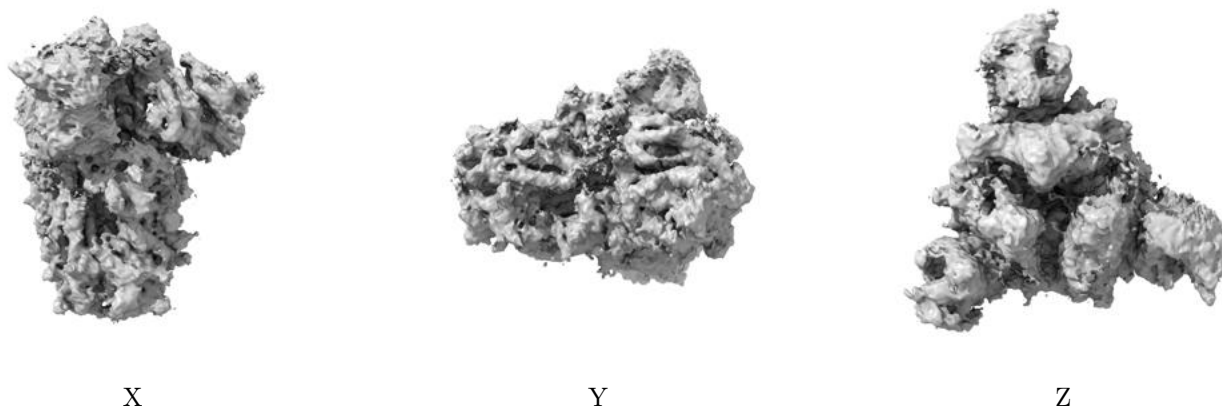
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

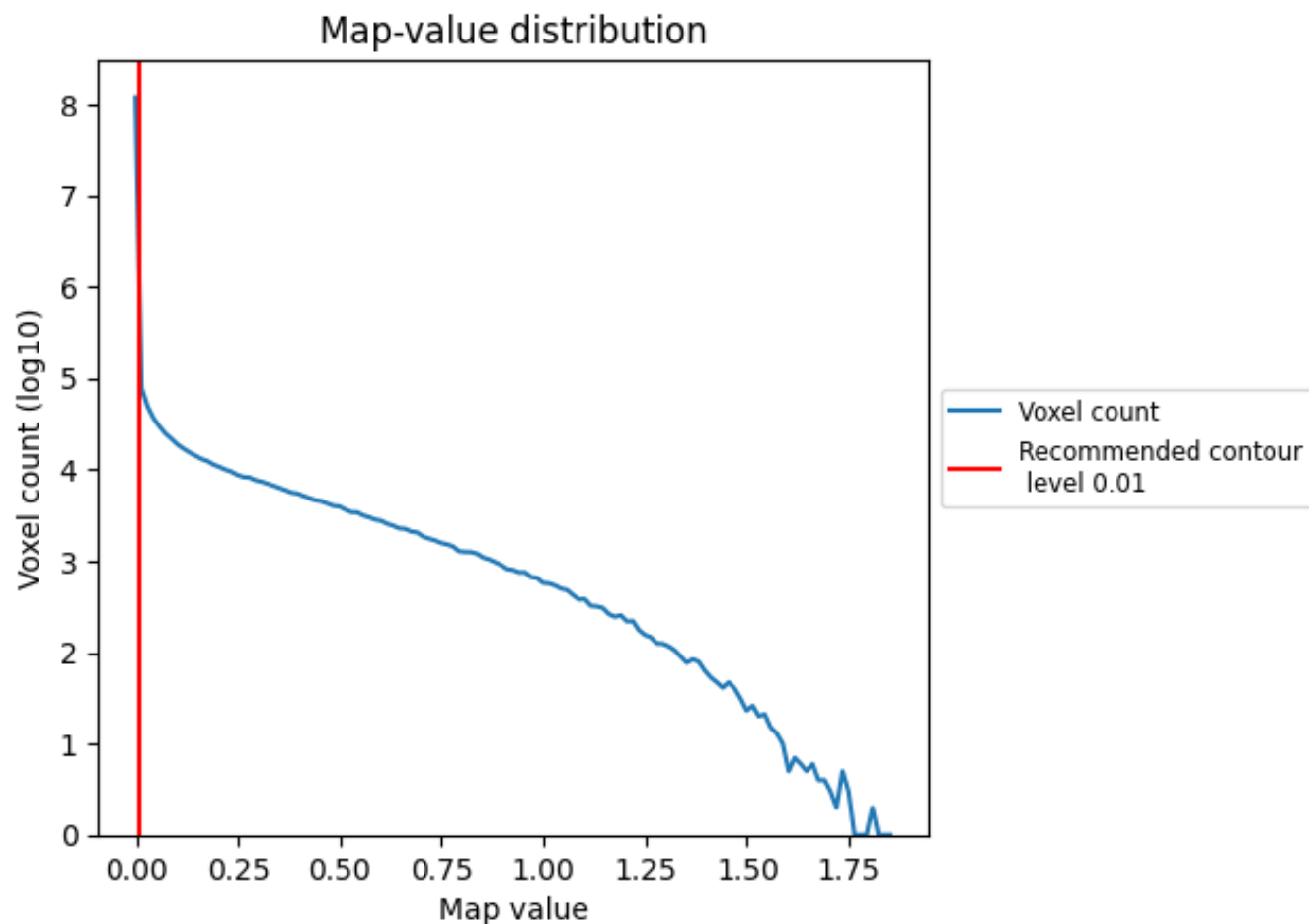
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

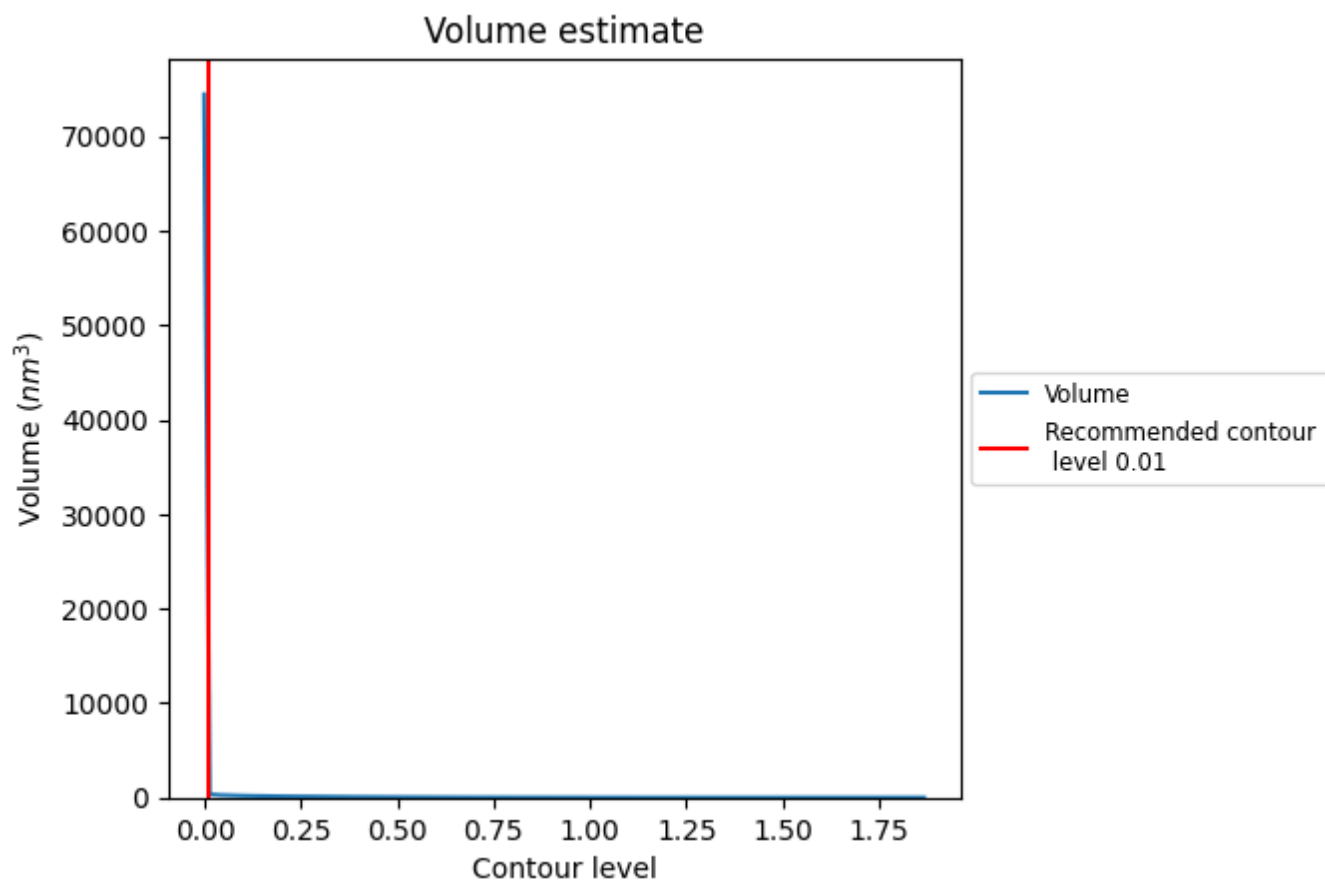
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

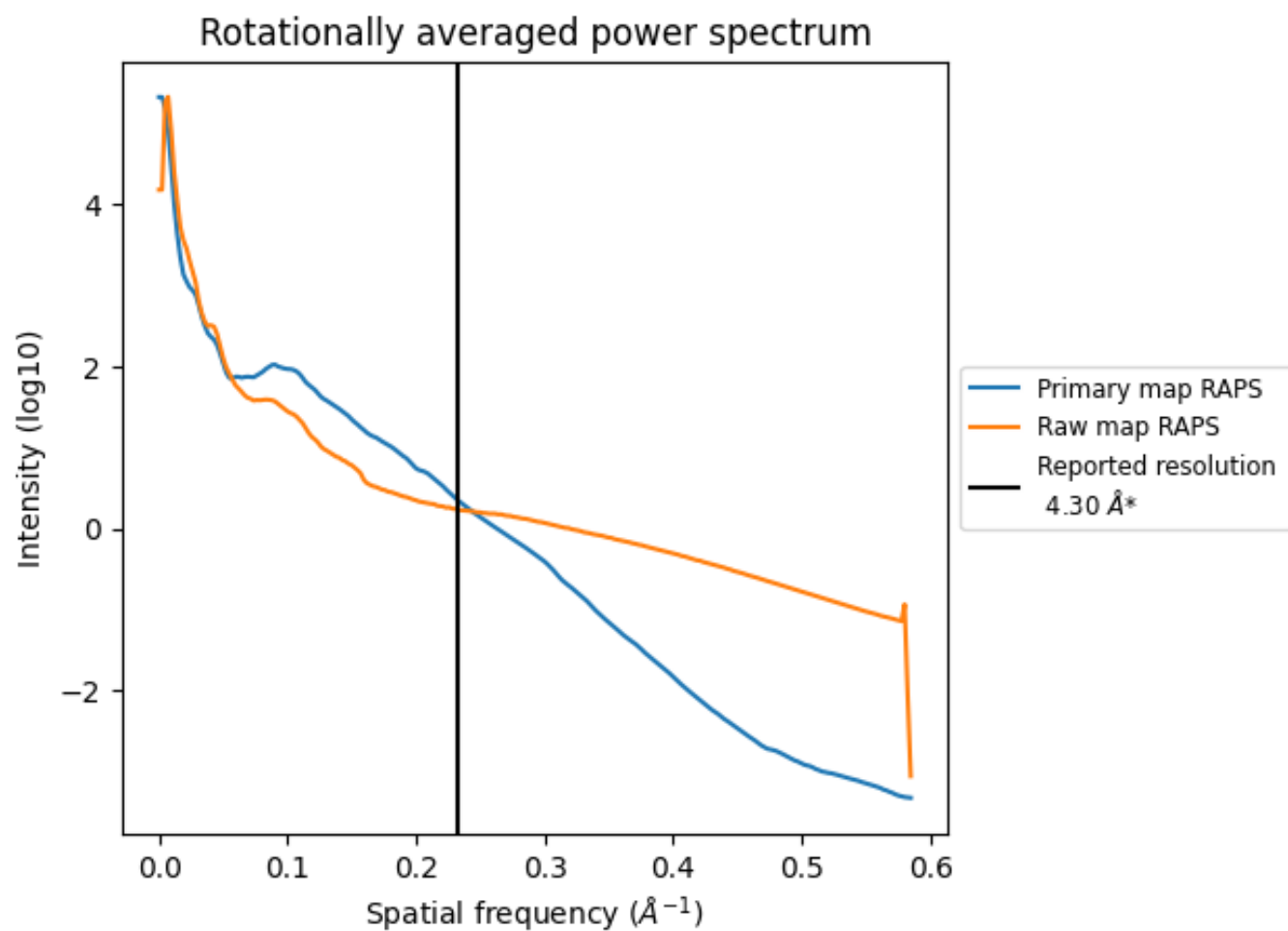
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15139 nm^3 ; this corresponds to an approximate mass of 13676 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

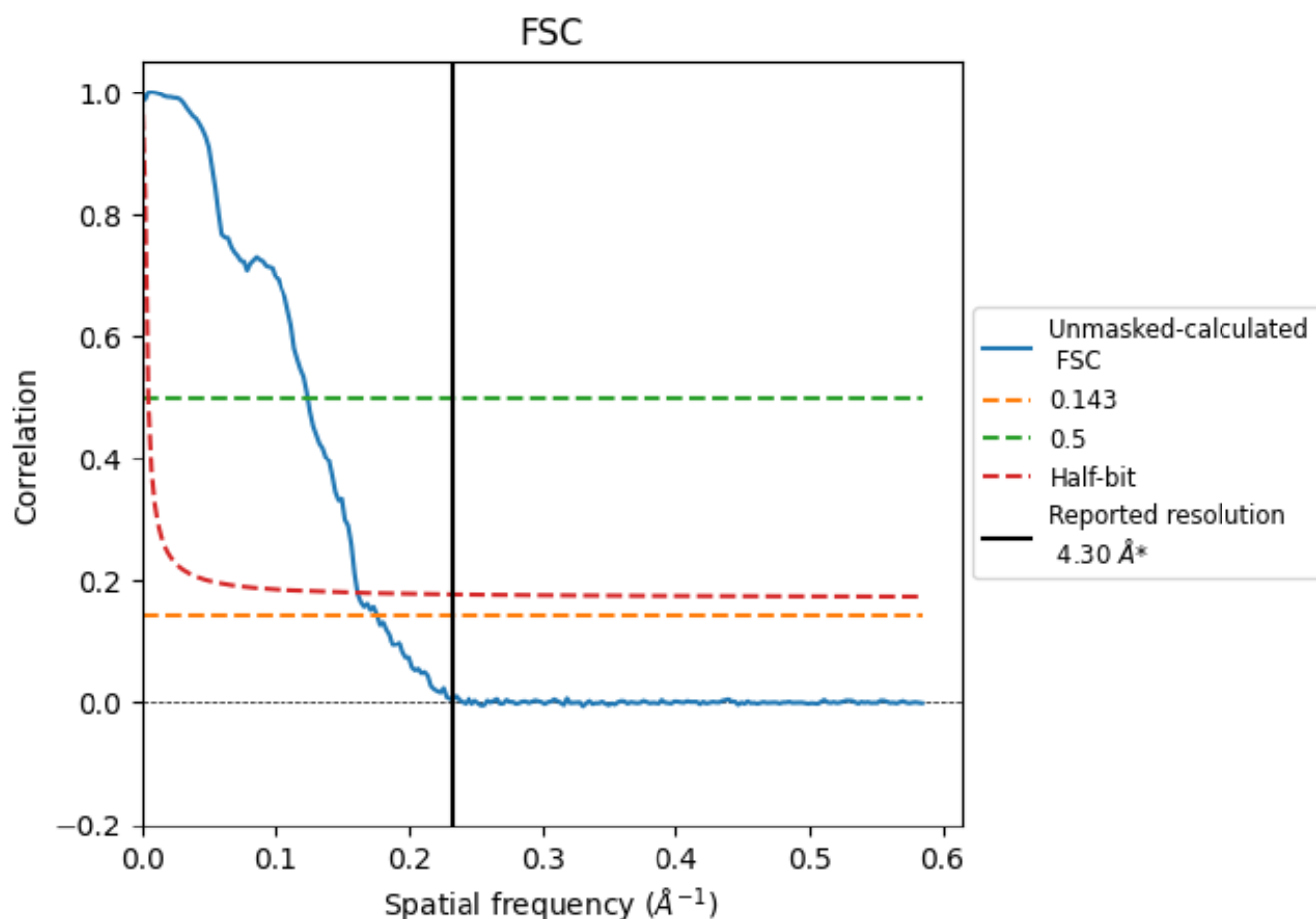


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

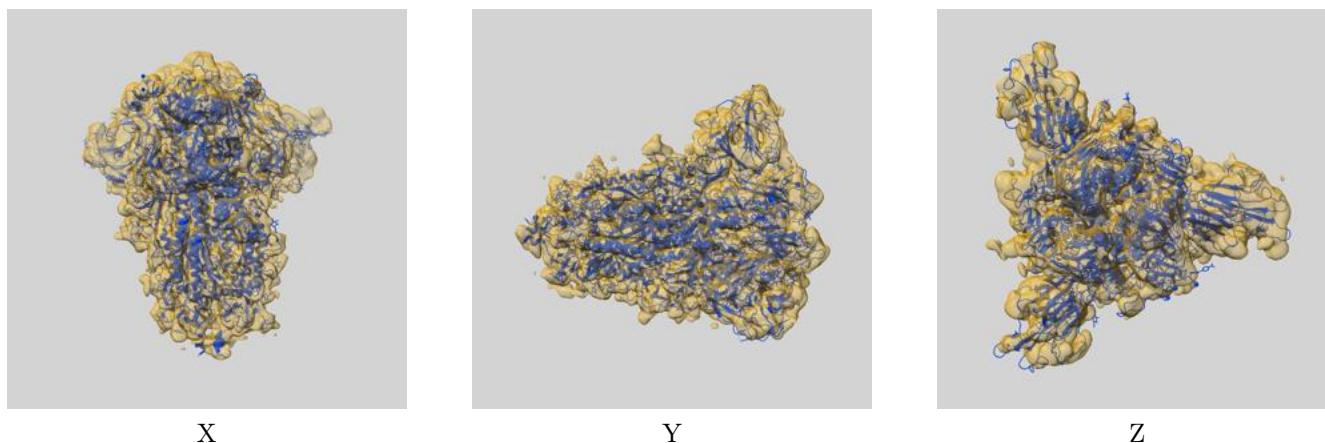
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.68	8.05	6.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.68 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17578 and PDB model 8P9Y. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



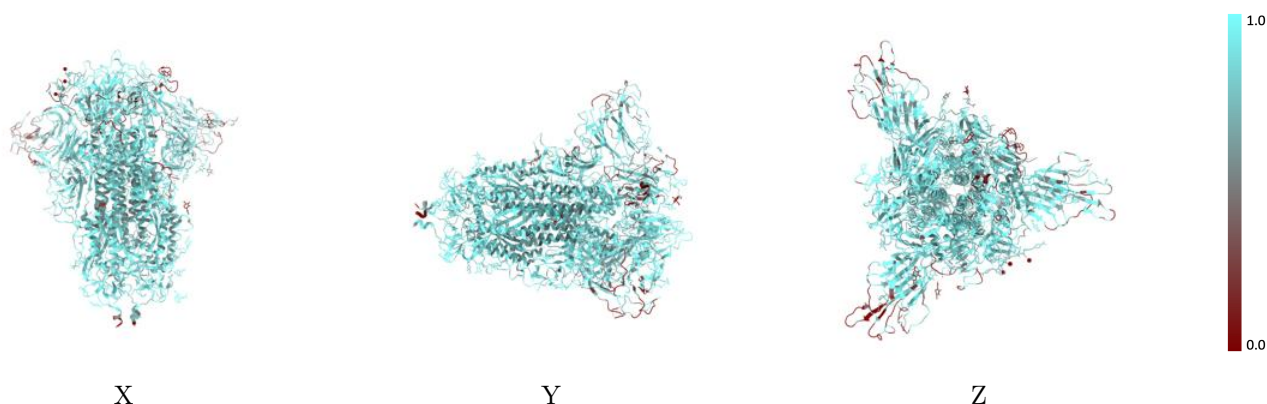
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



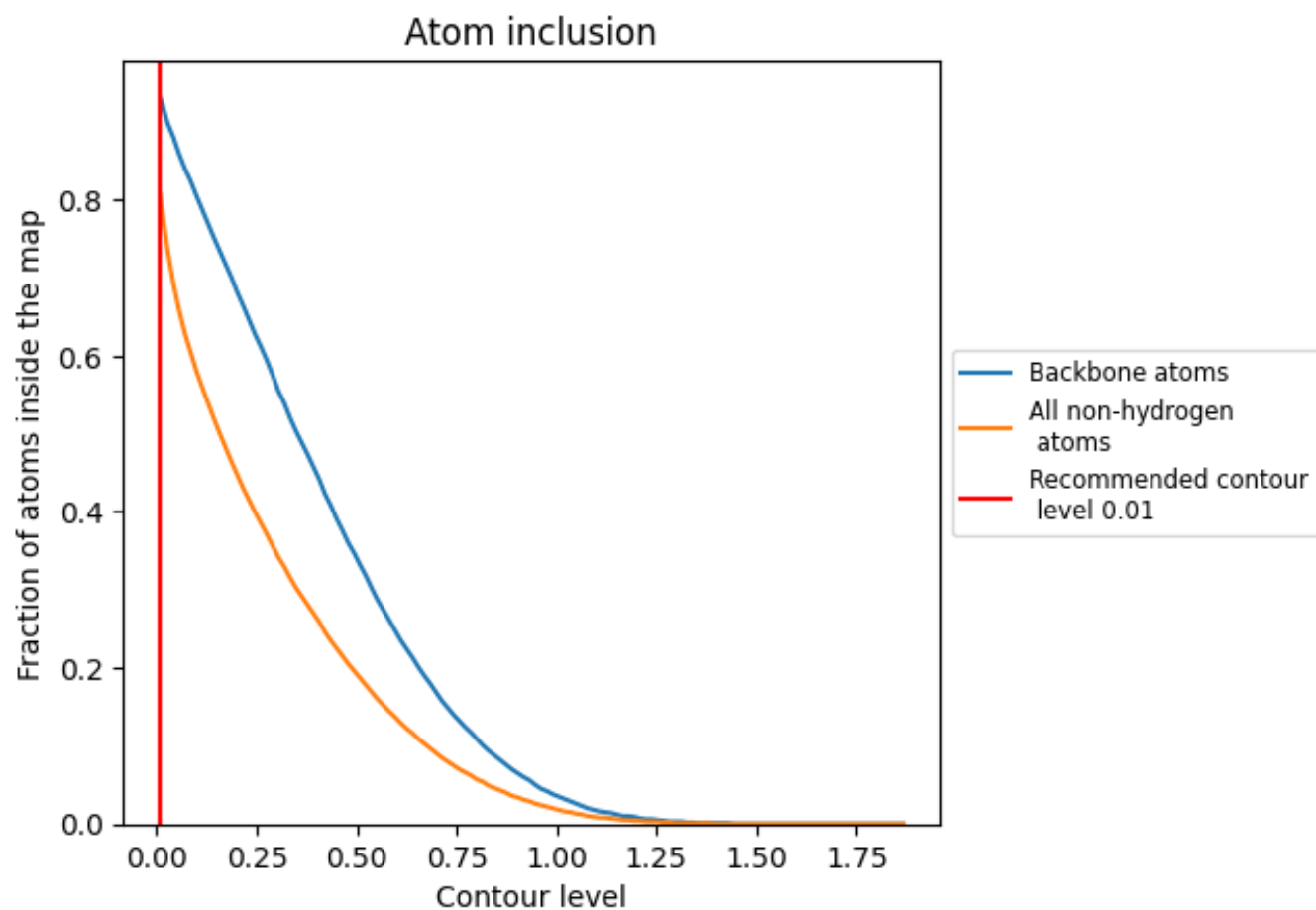
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.1170
A	 0.7830	 0.1110
B	 0.8340	 0.1200
C	 0.8070	 0.1170
D	 0.9640	 0.2830
E	 1.0000	 0.2490
F	 0.5710	 0.0870
G	 0.9290	 0.2820
H	 0.2860	 -0.0580
I	 1.0000	 0.2100
J	 0.4290	 0.0340
K	 0.8930	 0.2470
L	 0.6790	 0.1960
M	 1.0000	 0.2090

